

# Formally Biorthogonal Polynomials and a Look-ahead Levinson Algorithm for General Toeplitz Systems

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## ABSTRACT

Systems of linear equations with Toeplitz coefficient matrices arise in many important applications. The classical Levinson algorithm computes solutions of Toeplitz systems with only  $O(n^2)$  arithmetic operations, as compared to  $O(n^3)$  operations that are needed for solving general linear systems. However, the Levinson algorithm in its original form requires that all leading principal submatrices be nonsingular. In this paper, an extension of the Levinson algorithm to general Toeplitz systems is presented. The algorithm uses look-ahead to skip over exactly singular as well as ill-conditioned leading submatrices, and at the same time it still fully exploits the Toeplitz structure. In our derivation of this algorithm, we make use of the intimate connection of Toeplitz matrices with formally biorthogonal polynomials. In particular, the occurrence of singular or ill-conditioned submatrices corresponds to a breakdown

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or near-breakdown in the standard recurrence relations for biorthogonal polynomials. We present new general recurrence relations that connect successive pairs in any given subsequence of all existing formally biorthogonal polynomials. These recurrences then immediately lead to the proposed look-ahead Levinson algorithm for solving Toeplitz systems. Implementation details for this algorithm and operation counts are given. Numerical experiments for Toeplitz systems with ill-conditioned submatrices are reported.

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## 1. INTRODUCTION

Matrices whose entries are equal along each diagonal are called *Toeplitz matrices*. In particular, a general square Toeplitz matrix of order  $n + 1$  is of the form

$$T_n = [t_{i-j}]_{i,j=0,\dots,n} = \begin{bmatrix} t_0 & t_{-1} & t_{-2} & \cdots & t_{-n} \\ t_1 & t_0 & t_{-1} & \cdots & t_{-n+1} \\ t_2 & t_1 & t_0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & t_{-1} \\ t_n & t_{n-1} & \cdots & t_1 & t_0 \end{bmatrix}, \quad (1.1)$$

where the entries  $t_i$  are real or complex numbers. In this paper, we are concerned with the solution of systems of linear equations

$$T_n x_n = b_n \quad (1.2)$$

with Toeplitz coefficient matrices (1.1). The task of solving Toeplitz systems (1.2) arises in many important applications, such as time-series analysis [13, 30], linear prediction [21, 37], spectral estimation [23, 25], system identification [27, 28, 31], Padé approximation [6, 19], and statistics [20].

There are classical *fast* algorithms for solving (1.2) that exploit the Toeplitz structure and require only  $O(n^2)$  operations, as compared to  $O(n^3)$  operations for general linear systems. These algorithms implicitly compute either an *inverse* triangular factorization of  $T_n$  of the type

$$V_n^T T_n U_n = D_n, \quad (1.3)$$

or a triangular factorization of  $T_n$  of the form

$$T_n = V_n^T D_n U_n; \quad (1.4)$$

see, e.g., [12]. Here, in (1.3) and (1.4),  $U_n$  and  $V_n$  are unit upper triangular matrices, and  $D_n$  is a diagonal matrix. The class of fast Toeplitz solvers based on (1.3) includes the Levinson algorithm [36] and its variants [13, 44, 49, 50]. Toeplitz solvers based on (1.4) are intimately connected with the classical work of Schur [40, 32], and they are called *Schur-type* methods. Algorithms in this second class were proposed by Bareiss [2], Rissanen [39], and others; we refer the reader to [32] and the references given there.

Note that, for a nonsingular matrix  $T_n$ , triangular decompositions of the type (1.3) and (1.4) exist if, and only if, all leading principal submatrices of  $T_n$  are nonsingular. Indeed, all classical fast Toeplitz solvers require that  $T_n$  be *strongly regular*, i.e., the submatrices  $T_m$ ,  $m = 0, 1, \dots, n-1$ , must all be nonsingular. In some, but by far not all, applications that lead to Toeplitz systems the coefficient matrices  $T_n$  are Hermitian positive definite and thus guaranteed to be strongly regular. However, Hermitian indefinite and non-Hermitian Toeplitz matrices are in general not strongly regular, and it cannot be excluded that singular or ill-conditioned submatrices occur. We remark that Hermitian indefinite Toeplitz systems arise, for instance, in spectral estimation [38], when inverse iteration is used to compute eigenvalues of Hermitian positive definite Toeplitz matrices; see [10, 23, 25].

It is well known that the Levinson algorithm and the Schur-type Toeplitz solvers can be extended to handle exactly singular leading principal submatrices, and numerous algorithms have been proposed [11, 18, 21, 24, 41, 48]. These algorithms are again based on triangular factorizations of the type (1.3) or (1.4), where now  $D_n$  is a block-diagonal matrix. More precisely, blocks of size  $h_k \geq 1$  in  $D_n$  just correspond to  $h_k - 1$  consecutive singular leading submatrices of  $T_n$ .

In finite-precision arithmetic, it is not enough to skip only over exactly singular submatrices, and a numerically robust Toeplitz solver also must be able to handle nonsingular, yet ill-conditioned leading principal submatrices. The literature on Toeplitz algorithms with this property is rather scarce. Sweet [42, 43] showed that, in principle, pivoting can be incorporated into the Bareiss algorithm, which allows one to treat singular and nearly singular submatrices. However, there are some unresolved difficulties with this algorithm, such as the necessity for an *a priori* choice of parameters, and the fact that a large pivot does not necessarily guarantee well-conditioned submatrices. Recently, Chan and Hansen [9] proposed a look-ahead modification of the Levinson algorithm for general Toeplitz systems. If a singular or a

nonsingular ill-conditioned submatrix occurs, then the algorithm looks ahead to the next well-conditioned leading submatrix, and instead of a standard Levinson step, a block step is performed. However, this look-ahead algorithm is not entirely satisfactory. The look-ahead strategy used in [9] requires condition-number estimates for all leading submatrices, and this generates overhead of order  $O(n^2)$ , even if it turns out that no block steps are necessary. Moreover, as we will demonstrate with an example in Section 7.2 below, there is a potential source for a breakdown of the algorithm if two or more consecutive block steps are performed.

In this paper, we propose a look-ahead Levinson algorithm for general Toeplitz systems that is different from the one in [9]. In our derivation of this algorithm, we make use of the intimate connection of Toeplitz matrices with *formally biorthogonal polynomials* (FBOPs). In particular, the occurrence of singular or ill-conditioned submatrices corresponds to a breakdown or near-breakdown in the standard recurrence relations for biorthogonal polynomials. First, we derive new general recurrence relations that connect successive pairs in any given subsequence of all existing FBOPs. These recurrences then immediately lead to the proposed look-ahead Levinson algorithm for solving Toeplitz systems.

The remainder of this paper is organized as follows. In Section 2, we introduce some notation, and we give a formal definition of FBOPs associated with general bilinear forms. We then turn to bilinear forms induced by Toeplitz matrices, and in Section 3 we collect some basic properties of the corresponding FBOPs. In Section 4, we derive general recurrence relations for FBOPs. In Section 5, we propose a look-ahead procedure for constructing FBOPs, and we describe some properties of this algorithm. In Section 6, we present our look-ahead Levinson algorithm for solving general Toeplitz systems. We give implementation details and operation counts, and we discuss the look-ahead strategy. In Section 7, we consider the look-ahead Levinson algorithm for the special case of Hermitian Toeplitz systems. Also, we show that the procedure proposed by Chan and Hansen has potential breakdowns. In Section 8, we report results of numerical experiments with Toeplitz matrices that have various kinds of ill-conditioned submatrices. Finally, in Section 9, we make some concluding remarks.

## 2. PRELIMINARIES

In this section, we introduce some notation, and we give a formal definition of FBOPs associated with general bilinear forms.

### 2.1. Notation

Throughout the paper, all vectors and matrices are allowed to have complex entries. As usual,  $M^T := [m_{kj}]$ ,  $\bar{M} := [\bar{m}_{jk}]$ , and  $M^H := \bar{M}^T$  denote the transpose, complex conjugate, and conjugate transpose, respectively, of a matrix  $M = [m_{jk}]$ . The vector norm  $\|x\| := \sqrt{x^H x}$  is the Euclidean norm, and  $\|M\| := \max_{\|x\|=1} \|Mx\|$  is the corresponding matrix norm. For square matrices  $M \in \mathbb{C}^{h \times h}$ , we use the following condition number:

$$\kappa(M) := \begin{cases} 1/|M| & \text{if } h = 1, \\ \|M\| \cdot \|M^{-1}\| & \text{if } h > 1. \end{cases} \quad (2.1)$$

Whenever we call a square matrix *ill-conditioned*, it is with respect to the condition number (2.1). We denote by  $I_k \in \mathbb{R}^{k \times k}$  the  $k \times k$  identity matrix, by

$$J_k := \begin{bmatrix} 0 & \cdots & 0 & 1 \\ \vdots & \ddots & 1 & 0 \\ 0 & \ddots & \ddots & \vdots \\ 1 & 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{k \times k}$$

the  $k \times k$  antidiagonal identity matrix, by  $0_{k \times j}$  the  $k \times j$  zero matrix, and by  $0_k \in \mathbb{R}^k$  the zero vector of length  $k$ . We will drop subscripts and simply write  $I$ ,  $J$ , or  $0$  if the actual dimensions are apparent from the context.

The set of all complex polynomials of degree at most  $n$  is denoted by

$$\mathcal{P}_n := \{\varphi(\lambda) \equiv \sigma_0 + \sigma_1 \lambda + \cdots + \sigma_n \lambda^n \mid \sigma_0, \sigma_1, \dots, \sigma_n \in \mathbb{C}\},$$

and  $\mathcal{P}$  is the set of all complex polynomials. We denote by  $\partial(\varphi)$  the exact degree of  $\varphi \in \mathcal{P}$ , i.e.,  $\partial(\varphi)$  is the smallest integer  $n \geq 0$  such that  $\varphi \in \mathcal{P}_n$ . A polynomial  $\varphi \in \mathcal{P}_n$  is called *monic* if it is of exact degree  $n$  with leading coefficient 1. For each  $\varphi \in \mathcal{P}$ , we define its *reverse*  $\hat{\varphi}$  by

$$\hat{\varphi}(\lambda) \equiv \lambda^{\partial(\varphi)} \varphi(1/\lambda). \quad (2.2)$$

Note that  $\hat{\varphi}$  is a polynomial of degree at most  $\partial(\varphi)$ .

Capital Greek letters are always used to denote row vectors of polynomials in  $\mathcal{P}$ , e.g.,

$$\Phi = [\varphi_0 \quad \varphi_1 \quad \cdots \quad \varphi_j]. \quad (2.3)$$

A vector of the type (2.3) is called a *block* of polynomials. The *reverse*  $\hat{\Phi}$  of a block (2.3) is defined by

$$\hat{\Phi}(\lambda) \equiv \lambda^{n_\Phi} \Phi(1/\lambda), \quad \text{where } n_\Phi := \max_{i=0,1,\dots,j} \partial(\varphi_i). \quad (2.4)$$

Note that the entries of  $\hat{\Phi}$  are again polynomials, and

$$\hat{\Phi} = \begin{bmatrix} \lambda^{n_\Phi - \partial(\varphi_0)} \hat{\varphi}_0 & \lambda^{n_\Phi - \partial(\varphi_1)} \hat{\varphi}_1 & \dots & \lambda^{n_\Phi - \partial(\varphi_j)} \hat{\varphi}_j \end{bmatrix}. \quad (2.5)$$

Furthermore, if  $j = 0$  in (2.3), then (2.4) reduces to the usual reverse (2.2) of a single polynomial.

Finally, for each  $n$ , we denote by

$$\Lambda_n = \begin{bmatrix} 1 & \lambda & \lambda^2 & \dots & \lambda^n \end{bmatrix} \quad (2.6)$$

the block whose entries are the monomials  $\lambda^i$ ,  $i = 0, 1, \dots, n$ . We remark that, with (2.6) and  $n_\Phi$  from (2.4), any block (2.3) and its reverse can be represented in the form

$$\Phi = \Lambda_{n_\Phi} U \quad \text{and} \quad \hat{\Phi} = \Lambda_{n_\Phi} J U, \quad (2.7)$$

respectively. Here  $U \in \mathbb{C}^{(n_\Phi+1) \times (j+1)}$  is a matrix whose  $i$ th column just contains the coefficients of the polynomial  $\varphi_i$ ,  $i = 0, 1, \dots, j$ . In particular, each  $\varphi \in \mathcal{P}_n$  can be written in the form

$$\varphi = \Lambda_n u \quad \text{for some } u \in \mathbb{C}^{n+1}. \quad (2.8)$$

## 2.2. Bilinear Forms and FBOPs

A complex-valued functional

$$\langle \cdot, \cdot \rangle : \mathcal{P} \times \mathcal{P} \mapsto \mathbb{C} \quad (2.9)$$

is called a *bilinear form* if

$$\begin{aligned} \langle \psi, \sigma_1 \varphi_1 + \sigma_2 \varphi_2 \rangle &= \sigma_1 \langle \psi, \varphi_1 \rangle + \sigma_2 \langle \psi, \varphi_2 \rangle \\ &\text{for all } \psi, \varphi_1, \varphi_2 \in \mathcal{P}, \quad \sigma_1, \sigma_2 \in \mathbb{C}, \\ \langle \tau_1 \psi_1 + \tau_2 \psi_2, \varphi \rangle &= \tau_1 \langle \psi_1, \varphi \rangle + \tau_2 \langle \psi_2, \varphi \rangle \\ &\text{for all } \psi_1, \psi_2, \varphi \in \mathcal{P}, \quad \tau_1, \tau_2 \in \mathbb{C}. \end{aligned} \quad (2.10)$$

We stress that a bilinear form is not an inner product. Indeed, it is possible that a nonzero polynomial  $\varphi$  has “norm”  $\langle \varphi, \varphi \rangle = 0$  or  $\langle \varphi, \varphi \rangle < 0$ .

Nevertheless, it turns out to be useful to study polynomials that are orthogonal with respect to a given bilinear form (2.9). Next we give a definition of these *formally biorthogonal polynomials* (FBOPs).

**DEFINITION 2.1.** A monic polynomial  $\varphi_n \in \mathcal{P}_n$  is called a *right FBOP* [with respect to the bilinear form (2.9)] of degree  $n$  if

$$\langle \psi, \varphi_n \rangle = 0 \quad \text{for all } \psi \in \mathcal{P}_{n-1}. \quad (2.11)$$

A monic polynomial  $\psi_n \in \mathcal{P}_n$  is called a *left FBOP* [with respect to the bilinear form (2.9)] of degree  $n$  if

$$\langle \psi_n, \varphi \rangle = 0 \quad \text{for all } \varphi \in \mathcal{P}_{n-1}. \quad (2.12)$$

A right or left FBOP  $\varphi_n$  or  $\psi_n$  is said to be *regular* if it is uniquely determined by (2.11) or (2.12), respectively.

**REMARK.** In general, regular FBOPs need not exist for every degree  $n$ ; for instance, see Lemma 3.1 below.

**REMARK.** Biorthogonal polynomials have been studied in various settings; we refer the reader to [3, 6, 33, 34, 47] and the papers cited therein. The notation “formally biorthogonal polynomials” goes back at least to van Rossum [47]. However, almost all the literature is concerned with cases where regular FBOPs of every degree  $n$  are guaranteed to exist or are assumed to exist.

In the sequel, it will be convenient to use the following extension of the bilinear form (2.9) to blocks of polynomials of the type (2.3). For any blocks

$$\Phi = [\varphi_0 \quad \varphi_1 \quad \cdots \quad \varphi_j] \quad \text{and} \quad \Psi = [\psi_0 \quad \psi_1 \quad \cdots \quad \psi_k],$$

we define

$$\langle \Psi, \Phi \rangle := \begin{bmatrix} \langle \psi_0, \varphi_0 \rangle & \cdots & \langle \psi_0, \varphi_j \rangle \\ \vdots & & \vdots \\ \langle \psi_k, \varphi_0 \rangle & \cdots & \langle \psi_k, \varphi_j \rangle \end{bmatrix} \in \mathbb{C}^{(k+1) \times (j+1)}.$$

## 3. FBOPS ASSOCIATED WITH TOEPLITZ MATRICES

Let  $\{t_i\}_{i=-\infty}^{\infty}$  be a given biinfinite sequence<sup>1</sup> of real or complex numbers, and let

$$T_n = [t_{i-j}]_{i,j=0,\dots,n}, \quad n = 0, 1, \dots,$$

be the associated family of Toeplitz matrices (1.1). The sequence  $\{T_n\}_{n=0}^{\infty}$  induces a bilinear form  $\langle \psi, \varphi \rangle$  on  $\mathcal{P} \times \mathcal{P}$  as follows. Using the representation (2.8), for any two polynomials

$$\varphi = \Lambda_n u, \quad \psi = \Lambda_n v, \quad u, v \in \mathbb{C}^{n+1},$$

of degree at most  $n$ ,  $n = 0, 1, \dots$ , we set

$$\langle \psi, \varphi \rangle := v^T T_n u. \quad (3.1)$$

From now on, we assume that  $\langle \cdot, \cdot \rangle$  is the bilinear form defined by (3.1). Furthermore, the term FBOP always refers to formally biorthogonal polynomials with respect to this particular bilinear form.

Next, we list some properties of  $\langle \cdot, \cdot \rangle$ . For the monomials  $\varphi(\lambda) \equiv \lambda^j$  and  $\psi(\lambda) \equiv \lambda^i$ , we obtain

$$\langle \lambda^i, \lambda^j \rangle = t_{i-j}, \quad i, j = 0, 1, \dots, \quad (3.2)$$

and hence the elements of  $\{t_i\}_{i=-\infty}^{\infty}$  are just the *moments* associated with  $\langle \cdot, \cdot \rangle$ . From (3.2) and the bilinearity relations (2.10), it readily follows that

$$\langle \lambda \psi, \lambda \varphi \rangle = \langle \psi, \varphi \rangle \quad \text{for all } \varphi, \psi \in \mathcal{P}. \quad (3.3)$$

Furthermore, for all  $\varphi \in \mathcal{P}$  and all  $j, k = 0, 1, \dots$ , with  $\partial(\varphi) + k - j \geq 0$ , we have

$$\langle \lambda^k \hat{\varphi}, \lambda^j \rangle = \langle \lambda^{\partial(\varphi)+k-j}, \varphi \rangle, \quad (3.4)$$

$$\langle \lambda^j, \lambda^k \hat{\varphi} \rangle = \langle \varphi, \lambda^{\partial(\varphi)+k-j} \rangle. \quad (3.5)$$

<sup>1</sup>In the case that only a finite sequence  $t_{-n}, t_{-n+1}, \dots, t_n$  is given, we can always extend it to a biinfinite one, by simply setting  $t_i := t_{-i} := 0$  for all  $i > n$ .



For example, to verify (3.4), we set  $n := \partial(\varphi)$ , and we present  $\varphi, \hat{\varphi}$  in the form

$$\varphi(\lambda) \equiv \sum_{i=0}^n \sigma_i \lambda^i, \quad \hat{\varphi}(\lambda) \equiv \sum_{i=0}^n \sigma_i \lambda^{n-i}, \quad \text{with } \sigma_0, \sigma_1, \dots, \sigma_n \in \mathbb{C}.$$

Then, with (2.10) and (3.2), we obtain

$$\langle \lambda^k \hat{\varphi}, \lambda^j \rangle = \sum_{i=0}^n \sigma_i t_{(k+n-i)-j} = \sum_{i=0}^n \sigma_i t_{(n+k-j)-i} = \langle \lambda^{n+k-j}, \varphi \rangle.$$

Similarly, one can show (3.5).

In view of (2.11), (3.1), and (1.1), a polynomial

$$\varphi_n(\lambda) \equiv \lambda^n + \sum_{i=0}^{n-1} u_{in} \lambda^i$$

is a right FBOP of degree  $n$  if, and only if, its coefficients  $u_{in}$  satisfy

$$T_{n-1} \begin{bmatrix} u_{0n} \\ u_{1n} \\ \vdots \\ u_{n-1,n} \end{bmatrix} = - \begin{bmatrix} t_{-n} \\ t_{-(n-1)} \\ \vdots \\ t_{-1} \end{bmatrix}. \quad (3.6)$$

Analogously, by (2.12), (3.1), and (1.1), a polynomial

$$\psi_n(\lambda) \equiv \lambda^n + \sum_{i=0}^{n-1} v_{in} \lambda^i$$

is a left FBOP of degree  $n$  if, and only if, its coefficients  $v_{in}$  fulfill

$$\begin{bmatrix} v_{0n} & v_{1n} & \cdots & v_{n-1,n} \end{bmatrix} T_{n-1} = - \begin{bmatrix} t_n & t_{n-1} & \cdots & t_1 \end{bmatrix}. \quad (3.7)$$

As an immediate consequence of (3.6) and (3.7), we have the following result.

LEMMA 3.1. *The following conditions are equivalent:*

- (i) *A regular right FBOP  $\varphi_n$  of degree  $n$  exists.*
- (ii) *A regular left FBOP  $\psi_n$  of degree  $n$  exists.*
- (iii) *The matrix  $T_{n-1}$  is nonsingular.*

## 4. RECURRENCE RELATIONS FOR FBOPS

In general, regular FBOPs  $\varphi_n$  and  $\psi_n$  need not exist for every  $n$ . We denote by

$$\{n_j\}_{j=0}^J, \quad \text{where } 0 =: n_0 < n_1 < \cdots < n_j < \cdots, \quad (4.1)$$

the sequence of all integers  $n$  for which regular FBOPs of degree  $n$  exist. Here, either  $J = \infty$  or, if there are only finitely many regular FBOPs,  $J$  is an integer. We remark that, for  $n = 0$ , the conditions (3.6) and (3.7) are void, and thus  $\varphi_0(\lambda) \equiv 1$ ,  $\psi_0(\lambda) \equiv 1$  are regular FBOPs of degree 0. Hence  $n_0 = 0$  is always included in (4.1). Note that, in view of Lemma 3.1, the sequence  $\{n_j\}_{j=1}^J$  just consists of all integers  $n \geq 1$  for which  $T_{n-1}$  is nonsingular.

In this section, we derive recurrence relations for generating regular FBOPs corresponding to arbitrary subsequences of (4.1).

4.1. *The Classical Szegő Recursions*

If  $n_j \equiv j$  and thus regular FBOPs of degree  $n$  exist for every  $n$ , then they can be generated by means of the celebrated Szegő recursions [20, 3, 33].

ALGORITHM 4.1 (Szegő recursions).

(0) Set  $\varphi_0 = \psi_0 = 1$ ,  $\delta_0 = \langle 1, 1 \rangle$ .

For  $n = 0, 1, \dots$ , do:

(1) Compute  $\rho_n = \langle 1, \lambda \varphi_n \rangle$ ,  $\tau_n = \langle \lambda \psi_n, 1 \rangle$ .

(2) Set

$$\alpha_n = \rho_n / \delta_n, \quad \varphi_{n+1} = \lambda \varphi_n - \hat{\psi}_n \alpha_n, \quad (4.2)$$

$$\beta_n = \tau_n / \delta_n, \quad \psi_{n+1} = \lambda \psi_n - \hat{\varphi}_n \beta_n.$$

(3) Set

$$\delta_{n+1} = \delta_n (1 - \alpha_n \beta_n). \quad (4.3)$$

We remark that the  $\delta_n$ 's in (4.3) satisfy

$$\delta_n = \langle \psi_n, \varphi_n \rangle. \quad (4.4)$$

The Szegő recursions are no longer valid if regular FBOPs do not exist for every  $n$ . There are extensions of the relations (4.2) that connect consecutive pairs  $\varphi_{n_j}, \psi_{n_j}$  and  $\varphi_{n_{j+1}}, \psi_{n_{j+1}}$  in the sequence (4.1) of *all* existing regular FBOPs. For example, such recurrences are given in [24] and, for the special case of Hermitian Toeplitz matrices  $\{T_n\}_{n=0}^\infty$ , in [11]. These recursions immediately lead to an extension of the Levinson algorithm that can skip over exactly singular leading submatrices. For the derivation of a more robust Levinson algorithm that can also skip over nonsingular, but ill-conditioned submatrices, we need more general recurrence relations that connect consecutive pairs in a subsequence of all existing regular FBOPs. In the next section, we present such general recursions for FBOPs.

#### 4.2. General Recursions for FBOPs

Let  $\{n_{j_k}\}_{k=0}^K \subseteq \{n_j\}_{j=0}^J$  be an arbitrary, but fixed, subsequence of (4.1). Here either  $K = \infty$  or  $K$  is an integer. For simplicity, we set  $n_k := n_{j_k}$ . Moreover, in view of (4.1), we can assume that, without loss of generality,  $n_0 = 0$  is included in the subsequence. Therefore, we always have

$$0 =: n_0 < n_1 < \cdots < n_k < \cdots. \quad (4.5)$$

For all  $0 \leq k < K$ , we set

$$h_k := n_{k+1} - n_k \quad \text{and} \quad \mathcal{J}_k := \begin{cases} \emptyset & \text{if } h_k = 1, \\ \{n \mid n_k < n < n_{k+1}\} & \text{if } h_k > 1. \end{cases} \quad (4.6)$$

If  $K < \infty$ , then we set  $n_{K+1} := \infty$  and  $\mathcal{J}_K := \{n \mid n > n_K\}$ .

The goal then is to give recurrences for generating the regular FBOPs

$$\{\varphi_{n_k}\}_{k=0}^K \quad \text{and} \quad \{\psi_{n_k}\}_{k=0}^K \quad (4.7)$$

corresponding to the prescribed indices (4.5). To this end, we also construct additional monic polynomials

$$\varphi_n, \psi_n \in \mathcal{P}_n \quad \text{for all } n \in \mathcal{J}_k \quad \text{and all } k. \quad (4.8)$$

The polynomials (4.8) are called *inner* polynomials. Note that the regular FBOPs (4.7) together with the inner polynomials (4.8) build two sequences of monic polynomials  $\{\varphi_n\}_{n=0}^\infty$  and  $\{\psi_n\}_{n=0}^\infty$  that both span  $\mathcal{P}$ . Of course, we still need to specify how to actually choose the inner polynomials. In order to obtain recurrence relations that involve as few as possible previous polynomials, it is crucial to construct the inner polynomials  $\varphi_n, \psi_n$ ,  $n \in \mathcal{J}_k$ , as *quasi*-FBOPs, in the sense that they satisfy the relaxed biorthogonality relations

$$\begin{aligned}\langle \psi, \varphi_n \rangle &= 0 & \text{for all } \psi \in \mathcal{P}_{n_k-1}, \\ \langle \psi_n, \varphi \rangle &= 0 & \text{for all } \varphi \in \mathcal{P}_{n_k-1}.\end{aligned}\tag{4.9}$$

Next we introduce some further notation. For all  $0 \leq k < K$ , we define blocks of polynomials

$$\begin{aligned}\Phi^{(k)} &:= [\varphi_{n_k} \quad \varphi_{n_k+1} \quad \cdots \quad \varphi_{n_{k+1}-1}], \\ \Psi^{(k)} &:= [\psi_{n_k} \quad \psi_{n_k+1} \quad \cdots \quad \psi_{n_{k+1}-1}].\end{aligned}\tag{4.10}$$

If  $K < \infty$ , then we also define infinite row vectors of polynomials

$$\Phi^{(K)} := [\varphi_{n_K} \quad \varphi_{n_K+1} \quad \cdots], \quad \Psi^{(K)} := [\psi_{n_K} \quad \psi_{n_K+1} \quad \cdots].$$

Moreover, for all  $0 \leq k < K$ , we set

$$\Lambda^{(k)} := [\lambda^{n_k} \quad \lambda^{n_k+1} \quad \cdots \quad \lambda^{n_{k+1}-1}],\tag{4.11}$$

$$F^{(k)} := \langle \Lambda^{(k)}, \Phi^{(k)} \rangle, \quad G^{(k)} := \langle \Psi^{(k)}, \Lambda^{(k)} \rangle.\tag{4.12}$$

We remark that, with (4.11), the biorthogonality conditions (2.11) and (2.12) for the regular FBOPs (4.7) and the relaxed biorthogonality relations (4.9) for quasi-FBOPs can be summarized as follows: the polynomials  $\varphi_n, \psi_n$ ,  $n = 0, 1, \dots$ , are required to satisfy

$$\langle \Lambda^{(m)}, \varphi_n \rangle = 0 \text{ and } \langle \psi_n, \Lambda^{(m)} \rangle = 0 \quad \text{for all } m = 0, 1, \dots, k(n) - 1,\tag{4.13}$$

where  $k(n)$  is the integer such that  $n_{k(n)} \leq n < n_{k(n)+1}$ .

Note that  $F^{(k)}$  and  $G^{(k)}$  defined in (4.12) are  $h_k \times h_k$  matrices, with  $h_k$  from (4.6). We will need the fact that these matrices are nonsingular.

LEMMA 4.2. *If the inner polynomials (4.8) are constructed as quasi-FBOPs, then the matrices  $F^{(k)}$  and  $G^{(k)}$  are nonsingular for all  $0 \leq k < K$ .*

*Proof.* Suppose that  $F^{(k)}$  is singular. Then there exists a vector  $z \in \mathbb{C}^{h_k}$  such that

$$F^{(k)}z = 0 \quad \text{and} \quad z \neq 0, \quad (4.14)$$

and we set

$$\varphi := \varphi_{n_{k+1}} + \Phi^{(k)}z. \quad (4.15)$$

Clearly,  $\varphi$  is a monic polynomial of degree  $n_{k+1}$ , and since the polynomials in the block  $\Phi^{(k)}$  are linearly independent, we have  $\varphi \neq \varphi_{n_{k+1}}$ . Using (4.13)–(4.15), we deduce that

$$\begin{aligned} \langle \Lambda^{(m)}, \varphi \rangle &= \langle \Lambda^{(m)}, \varphi_{n_{k+1}} \rangle + \langle \Lambda^{(m)}, \Phi^{(k)} \rangle z \\ &= \begin{cases} 0 & \text{if } 0 \leq m < k, \\ F^{(k)}z = 0 & \text{if } m = k. \end{cases} \end{aligned}$$

Hence  $\varphi$  is a regular right FBOP of degree  $n_{k+1}$ , and this contradicts the uniqueness of regular FBOPs.

Similarly, one shows that  $G^{(k)}$  is nonsingular. ■

For the formulation of our recurrence relations, we will also need the following quantities. If  $h_k > 1$ , we define

$$\begin{aligned} f_k &:= \begin{bmatrix} I_{h_k-1} & 0_{h_k-1} \end{bmatrix} F^{(k)} \begin{bmatrix} 0_{h_k-1} \\ 1 \end{bmatrix}, \\ g_k &:= \begin{bmatrix} I_{h_k-1} & 0_{h_k-1} \end{bmatrix} (G^{(k)})^T \begin{bmatrix} 0_{h_k-1} \\ 1 \end{bmatrix}, \end{aligned} \quad (4.16)$$

and if  $h_k = 1$ , we set  $f_k = g_k = \emptyset$ . We remark that  $f_k$  and  $g_k$  just consist of the first  $h_k - 1$  elements of the last columns of  $F^{(k)}$  and  $(G^{(k)})^T$ , respec-

tively. Thus we have

$$F^{(k)} = \begin{bmatrix} * & f_k \\ * & * \end{bmatrix} \quad \text{and} \quad (G^{(k)})^T = \begin{bmatrix} * & g_k \\ * & * \end{bmatrix}, \quad (4.17)$$

where the elements  $*$  in the lower right corners in (4.17) are  $1 \times 1$ .

After these preparations, we can now state our recurrence relations for generating the regular FBOPs (4.7) corresponding to the prescribed indices (4.5), together with inner polynomials (4.8) satisfying the relaxed biorthogonality conditions (4.9). First, we set  $\varphi_{-1} = \psi_{-1} = \lambda^{-1}$  and  $\Phi^{(-1)} = \Psi^{(-1)} = \emptyset$ . Then, for all  $-1 \leq k < K$  and  $n_{k+1} \leq n+1 < n_{k+2}$ , we set

$$\varphi_{n+1} = \lambda \varphi_n - \hat{\Psi}^{(k)} \alpha_n - \begin{cases} \Phi^{(k)} \mu_n & \text{if } n+1 = n_{k+1}, \\ \sum_{i=n_{k+1}}^n \xi_i^{(n)} \varphi_i & \text{if } n+1 \in \mathcal{J}_{k+1}, \end{cases} \quad (4.18)$$

where

$$\alpha_n = (G^{(k)})^{-T} \begin{bmatrix} 0_{h_k-1} \\ \rho_n \end{bmatrix}, \quad \rho_n = \langle 1, \lambda \varphi_n \rangle, \quad \mu_n = (F^{(k)})^{-1} \begin{bmatrix} 0 \\ f_k \end{bmatrix}, \quad (4.19)$$

and

$$\psi_{n+1} = \lambda \psi_n - \hat{\Phi}^{(k)} \beta_n - \begin{cases} \Psi^{(k)} \nu_n & \text{if } n+1 = n_{k+1}, \\ \sum_{i=n_{k+1}}^n \zeta_i^{(n)} \psi_i & \text{if } n+1 \in \mathcal{J}_{k+1}, \end{cases} \quad (4.20)$$

where

$$\beta_n = (F^{(k)})^{-1} \begin{bmatrix} 0_{h_k-1} \\ \tau_n \end{bmatrix}, \quad \tau_n = \langle \lambda \psi_n, 1 \rangle, \quad \nu_n = (G^{(k)})^{-T} \begin{bmatrix} 0 \\ g_k \end{bmatrix}. \quad (4.21)$$

Here, in (4.18) and (4.20),  $\xi_i^{(n)}, \zeta_i^{(n)} \in \mathbb{C}$  are coefficients that can be chosen arbitrarily.

Note that, by Lemma 4.2, the inverse matrices in (4.19) and (4.21) all exist. Moreover, we remark that the recurrence (4.20) can be equivalently formulated in terms of the reverse polynomials that appear in (4.18). The resulting relation is as follows:

$$\hat{\psi}_{n+1} = \hat{\psi}_n - \lambda^{n+2-n_{k+1}} \Phi^{(k)} \beta_n - \begin{cases} \lambda \hat{\Psi}^{(k)} \nu_n & \text{if } n+1 = n_{k+1}, \\ \sum_{i=n_{k+1}}^n \zeta_i^{(n)} \lambda^{n+1-i} \hat{\psi}_i & \text{if } n+1 \in \mathcal{J}_{k+1}. \end{cases}$$

Of course, we still need to verify that the recursions (4.18)–(4.21) indeed generate the regular FBOPs (4.7).

**THEOREM 4.3.** *Let  $\{\varphi_n\}_{n=0}^\infty$  and  $\{\psi_n\}_{n=0}^\infty$  be the sequences of polynomials defined by the recurrence relations (4.18)–(4.21). Then these polynomials satisfy the biorthogonality relations (4.13). In particular, the polynomials  $\{\varphi_n\}_{n=0}^K$  and  $\{\psi_n\}_{n=0}^K$  are the uniquely defined regular FBOPs corresponding to the prescribed indices (4.5).*

*Proof.* We show (4.13) by induction on  $n$ . For  $n = 0$ , by (4.5),  $k(0) = 0$ , and the conditions (4.13) are void.

Now let  $n \geq 0$ , and assume that (4.13) holds for all polynomials  $\varphi_0, \varphi_1, \dots, \varphi_n$  and  $\psi_0, \psi_1, \dots, \psi_n$ . We need to show that  $\varphi_{n+1}$  and  $\psi_{n+1}$  satisfy

$$\langle \lambda^j, \varphi_{n+1} \rangle = 0 \quad \text{for all } j = 0, 1, \dots, n_{k+1} - 1, \quad (4.22)$$

and

$$\langle \psi_{n+1}, \lambda^j \rangle = 0 \quad \text{for all } j = 0, 1, \dots, n_{k+1} - 1, \quad (4.23)$$

respectively. Here  $k$  is the integer defined by  $n_{k+1} \leq n+1 < n_{k+2}$ . To simplify notation, we set  $h' := h_k - 1$  and  $n' := n_{k+1} - 1$ . Moreover, in the following, we always assume that  $j \in \{0, 1, \dots, n'\}$ .

First, we consider (4.22). Writing  $\hat{\Psi}^{(k)}$  in the form (2.5) and using (3.5), one readily verifies that

$$\langle \lambda^j, \hat{\Psi}^{(k)} \rangle = \langle \Psi^{(k)}, \lambda^{n'-j} \rangle^T. \quad (4.24)$$

From (4.24) and (4.13), it follows that

$$\langle \lambda^j, \hat{\Psi}^{(k)} \rangle = 0 \quad \text{for all } j \text{ with } h' < j \leq n'. \quad (4.25)$$

Using notation introduced in (2.6), (4.11), and (4.12), we can summarize (4.24) for the remaining indices  $0 \leq j \leq h'$  as follows:

$$\langle \Lambda_{h'}, \hat{\Psi}^{(k)} \rangle = \langle \Psi^{(k)}, \Lambda^{(k)} J \rangle^T = J(G^{(k)})^T. \quad (4.26)$$

Next, we note that, in view of (3.3) and (4.13), we have

$$\langle \lambda^j, \lambda \varphi_n \rangle = \begin{cases} \langle 1, \lambda \varphi_n \rangle = \rho_n & \text{if } j = 0, \\ \langle \lambda^{j-1}, \varphi_n \rangle = 0 & \text{if } 1 \leq j \leq n' \text{ and } n+1 \in \mathcal{J}_{k+1}, \\ \langle \lambda^{j-1}, \varphi_n \rangle = 0 & \text{if } 1 \leq j \leq n_k \text{ and } n+1 = n_{k+1}, \\ \langle \lambda^{j-1}, \varphi_n \rangle & \text{if } n_k < j \leq n' \text{ and } n+1 = n_{k+1}. \end{cases} \quad (4.27)$$

Using the vector  $f_k$  defined by (4.16) and (4.12), we can summarize the relations (4.27) for  $n_k \leq j \leq n'$  and  $n+1 = n_{k+1}$  as follows:

$$\langle \Lambda^{(k)}, \lambda \varphi_n \rangle = \begin{bmatrix} 0 \\ f_k \end{bmatrix}, \quad \text{if } n+1 = n_{k+1}. \quad (4.28)$$

With these preparations, it now readily follows that  $\varphi_{n+1}$  satisfies (4.22). With (4.18) and (4.13), we obtain

$$\begin{aligned} \langle \lambda^j, \varphi_{n+1} \rangle &= \langle \lambda^j, \lambda \varphi_n \rangle - \langle \lambda^j, \hat{\Psi}^{(k)} \rangle \alpha_n \\ &\quad - \begin{cases} \langle \lambda^j, \Phi^{(k)} \rangle \mu_n & \text{if } n+1 = n_{k+1}, \\ 0 & \text{if } n+1 \in \mathcal{J}_{k+1}. \end{cases} \end{aligned} \quad (4.29)$$

By (4.27), (4.25), and (4.13), all terms on the right-hand side of (4.29) vanish, and hence  $\langle \lambda^j, \varphi_{n+1} \rangle = 0$  for all  $j$  in the range  $h' < j < n_k$ , if  $n+1 = n_{k+1}$ , and for all  $j$  in the range  $h' < j \leq n'$ , if  $n+1 \in \mathcal{J}_{n+1}$ . For  $j$  in the range  $0 \leq j \leq h'$ , we use (4.29), (4.13), (4.27), (4.26), and the definition of  $\alpha_n$  in



(4.19) to deduce that

$$\langle \Lambda_{h'}, \varphi_{n+1} \rangle = \begin{bmatrix} \rho_n \\ 0_{h'} \end{bmatrix} - J(G^{(k)})^T \alpha_n = 0.$$

For the case that  $n + 1 = n_{k+1}$ , it remains to prove (4.22) for all  $j$  in the range  $n_k \leq j \leq n'$ . Here we use (4.29), (4.28), (4.25), (4.12), and the definition of  $\mu_n$  in (4.19) to verify that

$$\langle \Lambda^{(k)}, \varphi_{n+1} \rangle = \begin{bmatrix} 0 \\ f_k \end{bmatrix} - \langle \Lambda^{(k)}, \Phi^{(k)} \rangle \mu_n = \begin{bmatrix} 0 \\ f_k \end{bmatrix} - F^{(k)} \mu_n = 0.$$

This concludes the proof of (4.22).

To show (4.23) we proceed similarly. First, using (3.4) and (4.13), one verifies the relations

$$\begin{aligned} \langle \hat{\Phi}^{(k)}, \Lambda_{h'} \rangle &= (F^{(k)})^T J, \\ \langle \hat{\Phi}^{(k)}, \lambda^j \rangle &= 0 \quad \text{for all } j \text{ with } h' < j \leq n'. \end{aligned} \quad (4.30)$$

With (3.3) and (4.13), we obtain

$$\langle \lambda \psi_n, \lambda^j \rangle = \begin{cases} \langle \lambda \psi_n, 1 \rangle = \tau_n & \text{if } j = 0, \\ 0 & \text{if } 1 \leq j \leq n' \text{ and } n + 1 \in \mathcal{J}_{k+1}, \\ 0 & \text{if } 1 \leq j \leq n_k \text{ and } n + 1 = n_{k+1}, \end{cases} \quad (4.31)$$

$$\langle \lambda \psi_n, \Lambda^{(k)} \rangle = \begin{bmatrix} 0 & g_k^T \end{bmatrix} \quad \text{if } n + 1 = n_{k+1}. \quad (4.32)$$

Here  $g_k$  is the vector defined by (4.16) and (4.12). From (4.20) and (4.13), we have

$$\begin{aligned} \langle \psi_{n+1}, \lambda^j \rangle &= \langle \lambda \psi_n, \lambda^j \rangle - \beta_n^T \langle \hat{\Phi}^{(k)}, \lambda^j \rangle \\ &\quad - \begin{cases} \nu_n^T \langle \Psi^{(k)}, \lambda^j \rangle & \text{if } n + 1 = n_{k+1}, \\ 0 & \text{if } n + 1 \in \mathcal{J}_{k+1}. \end{cases} \end{aligned} \quad (4.33)$$

Finally, using (4.30)–(4.33) and the definitions of  $\beta_n$  and  $\nu_n$  in (4.21), one easily verifies (4.23). ■

REMARK. Our derivation of general recurrence relations is different from the one used in [24, 11] to obtain special recursions for all existing FBOPs. The approach in [24, 11] is based on Iohvidov's results [26] on the structure of exactly singular Toeplitz matrices, and it cannot be directly used to prove general recurrences of the type (4.18)–(4.21).

## 5. AN ALGORITHM FOR CONSTRUCTING FBOPS

In this section, we propose an algorithm for constructing regular FBOPs based on the general recurrence relations derived in Section 4.2, and we describe some properties of this algorithm. We use the notation introduced in Section 4.2.

### 5.1. The Algorithm

The algorithm generates two sequences  $\{\varphi_n\}_{n=0}^\infty$  and  $\{\psi_n\}_{n=0}^\infty$  of monic polynomials, where, for each  $n$ ,  $\varphi_n$  and  $\psi_n$  are either regular FBOPs or inner quasi-FBOPs. As in (4.5), we use the indices  $n_k$ ,  $k = 0, 1, \dots$ , to mark the regular FBOPs, and we always set  $n_0 = 0$ ,  $\varphi_0 = \psi_0 = 1$ . The index  $n = 0, 1, \dots$ , is used as an iteration counter, where in the course of the  $n$ th iteration the algorithm generates the next pair of polynomials  $\varphi_{n+1}$  and  $\psi_{n+1}$ . For each fixed  $n$ , we define  $l = l(n)$  by

$$n_l \leq n < n_{l+1}. \quad (5.1)$$

Note that  $l = l(n)$  is just the number of the last pair of regular FBOPs  $\varphi_{n_l}$  and  $\psi_{n_l}$  with degree  $\leq n$ . In addition to the blocks  $\Phi^{(k)}, \Psi^{(k)}$ ,  $k = 0, 1, \dots, l-1$ , defined in (4.10), we set

$$\Phi^{(l)} := [\varphi_{n_l} \quad \varphi_{n_l+1} \quad \cdots \quad \varphi_n], \quad \Psi^{(l)} := [\psi_{n_l} \quad \psi_{n_l+1} \quad \cdots \quad \psi_n]. \quad (5.2)$$

We call the blocks  $\Phi^{(l)}$  and  $\Psi^{(l)}$  *complete* if  $n+1 = n_{l+1}$ ; in this case, the next polynomials  $\varphi_{n+1}$  and  $\psi_{n+1}$  are constructed as regular FBOPs. If  $n+1 < n_{l+1}$ , then the blocks (5.2) are still *incomplete*; in this case, the next

polynomials  $\varphi_{n+1}$  and  $\psi_{n+1}$  are constructed as inner quasi-FBOPs and added to  $\Phi^{(l)}$  and  $\Psi^{(l)}$ , respectively. Finally, as in (4.11), (4.12), we set

$$\begin{aligned}\Lambda^{(l)} &:= [\lambda^{n_l} \quad \lambda^{n_l+1} \quad \dots \quad \lambda^n], \quad F^{(l)} := \langle \Lambda^{(l)}, \Phi^{(l)} \rangle, \\ G^{(l)} &:= \langle \Psi^{(l)}, \Lambda^{(l)} \rangle.\end{aligned}\quad (5.3)$$

Using this notation, we can rewrite the recurrences (4.18)–(4.21) in the form of the following algorithm.

ALGORITHM 5.1 (Construction of FBOPs).

(0) Set  $\varphi_0 = \psi_0 = 1$ ,  $\Phi^{(0)} = \Psi^{(0)} = 1$ ,  $F^{(0)} = G^{(0)} = \langle 1, 1 \rangle$ ,  $n_0 = 0$ ,  $l = 0$ .

For  $n = 0, 1, \dots$ , do:

(1) Compute

$$\rho_n = \langle 1, \lambda \varphi_n \rangle \quad \text{and} \quad \tau_n = \langle \lambda \psi_n, 1 \rangle. \quad (5.4)$$

(2) Decide whether to construct  $\varphi_{n+1}$  and  $\psi_{n+1}$  as regular FBOPs or as inner polynomials, and go to (3) or (4), respectively.

(3) (Regular step.) Set

$$\begin{aligned}\alpha_n &= (G^{(l)})^{-T} \begin{bmatrix} 0 \\ \rho_n \end{bmatrix}, \quad \mu_n = (F^{(l)})^{-1} \begin{bmatrix} 0 \\ f_l \end{bmatrix}, \\ \varphi_{n+1} &= \lambda \varphi_n - \hat{\Psi}^{(l)} \alpha_n - \Phi^{(l)} \mu_n,\end{aligned}\quad (5.5)$$

$$\begin{aligned}\beta_n &= (F^{(l)})^{-1} \begin{bmatrix} 0 \\ \tau_n \end{bmatrix}, \quad \nu_n = (G^{(l)})^{-T} \begin{bmatrix} 0 \\ g_l \end{bmatrix}, \\ \psi_{n+1} &= \lambda \psi_n - \hat{\Phi}^{(l)} \beta_n - \Psi^{(l)} \nu_n.\end{aligned}\quad (5.6)$$

Set  $n_{l+1} = n + 1$ ,  $l = l + 1$ ,  $\Phi^{(l)} = \Psi^{(l)} = \emptyset$ , and go to (5).

(4) (Inner step.) Set

$$\alpha_n = (G^{(l-1)})^{-T} \begin{bmatrix} 0 \\ \rho_n \end{bmatrix}, \quad \varphi_{n+1} = \lambda \varphi_n - \hat{\Psi}^{(l-1)} \alpha_n - \sum_{i=n_l}^n \xi_i^{(n)} \varphi_i, \quad (5.7)$$

$$\beta_n = (F^{(l-1)})^{-1} \begin{bmatrix} 0 \\ \tau_n \end{bmatrix}, \quad \psi_{n+1} = \lambda \psi_n - \hat{\Phi}^{(l-1)} \beta_n - \sum_{i=n_l}^n \zeta_i^{(n)} \psi_i. \quad (5.8)$$

(5) Set  $\Phi^{(l)} = [\Phi^{(l)} \varphi_{n+1}]$ ,  $\Psi^{(l)} = [\Psi^{(l)} \psi_{n+1}]$ ,  $F^{(l)} = \langle \Lambda^{(l)}, \Phi^{(l)} \rangle$ ,  $G^{(l)} = \langle \Psi^{(l)}, \Lambda^{(l)} \rangle$ .

Note that the description of Algorithm 5.1 is still incomplete, since no criteria for the decision in step (2) are given. We defer a discussion of this so-called *look-ahead strategy* to Section 6.3. Here, we only remark that, in view of Lemma 4.2, the polynomials  $\varphi_{n+1}$  and  $\psi_{n+1}$  can be constructed as regular FBOPs only if the following necessary condition holds true:

$$F^{(l)} \text{ and } G^{(l)} \text{ are nonsingular} \quad \text{if } n+1 = n_{l+1}. \quad (5.9)$$

In particular, (5.9) guarantees that the inverse matrices in (5.5)–(5.8) all exist.

### 5.2. Inverse Block-Factorization of Toeplitz Matrices

Next, we show that Algorithm 5.1 yields a factorization of  $T_n$  of the form (1.3), where  $D_n$  is now a block-diagonal matrix. In the following, let  $n \geq 0$  be arbitrary, but fixed, and let  $l = l(n)$  be the corresponding index defined by (5.1).

Recall that, by Theorem 4.3, the polynomials

$$\{\varphi_j\}_{j=0}^n \quad \text{and} \quad \{\psi_j\}_{j=0}^n \quad (5.10)$$

satisfy the conditions (4.13), which are equivalent to the following block-biorthogonality relations:

$$\langle \Psi^{(k)}, \Phi^{(m)} \rangle = 0 \quad \text{for all } k \neq m, \quad k, m = 0, 1, \dots, l. \quad (5.11)$$

Moreover, we set

$$D^{(k)} := \langle \Psi^{(k)}, \Phi^{(k)} \rangle, \quad k = 0, 1, \dots, l. \quad (5.12)$$

Here, in (5.11) and (5.12),  $\Psi^{(k)}$  and  $\Phi^{(k)}$  are the blocks defined in (4.10) if  $k < l$ , and in (5.2) if  $k = l$ . In view of (2.8), the monic polynomials (5.10) can

be represented in the form

$$\varphi_j = \Lambda_j u_j, \quad \text{where} \quad u_j := \begin{bmatrix} u_{0j} \\ u_{1j} \\ \vdots \\ u_{j-1,j} \\ 1 \end{bmatrix} \in \mathbb{C}^{j+1}, \quad (5.13)$$

$$\psi_j = \Lambda_j v_j, \quad \text{where} \quad v_j := \begin{bmatrix} v_{0j} \\ v_{1j} \\ \vdots \\ v_{j-1,j} \\ 1 \end{bmatrix} \in \mathbb{C}^{j+1}.$$

Using (5.13) and the definition of  $\langle \cdot, \cdot \rangle$  in (3.1), we can rewrite the relations (5.11) and (5.12) in the following matrix formulation:

$$V_n^T T_n U_n = D_n, \quad (5.14)$$

where

$$U_n := [u_{ij}]_{i,j=0,\dots,n} = \begin{bmatrix} 1 & u_{01} & \cdots & u_{0n} \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 \end{bmatrix} \quad (5.15)$$

and

$$V_n := [v_{ij}]_{i,j=0,\dots,n} = \begin{bmatrix} 1 & v_{01} & \cdots & v_{0n} \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 \end{bmatrix} \quad (5.16)$$

are unit upper triangular matrices, and

$$D_n := \text{diag}(D^{(0)}, D^{(1)}, \dots, D^{(l)}) \quad (5.17)$$

is a block-diagonal matrix. In other words, Algorithm 5.1 generates an inverse block-factorization (5.14) of  $T_n$ , where the columns of  $U_n$  and  $V_n$  are just the coefficients of the polynomials (5.10). Furthermore, the sizes of the blocks in (5.17) are given by

$$D^{(k)} \in \mathbb{C}^{h_k \times h_k}, \quad \text{where } h_k = \begin{cases} n_{k+1} - n_k & \text{if } 0 \leq k < l, \\ n + 1 - n_l & \text{if } k = l. \end{cases} \quad (5.18)$$

In particular,  $h_k = 1$  for all  $k$  if only regular steps (3) are performed in Algorithm 5.1. In the sequel, the construction of a *true* block of size  $h_k > 1$  will be referred to as a *look-ahead step*, and  $h_k$  will be called the *length* of the look-ahead step.

Finally, we remark that, by (5.13), the blocks  $\Phi^{(k)}$  and  $\Psi^{(k)}$  have the following representations:

$$\begin{aligned} \Phi^{(k)} &= \Lambda_{n_{k+1}-1} U^{(k)}, & \text{where } U^{(k)} &:= [u_{ij}]_{i=0, \dots, n_{k+1}-1; j=n_k, \dots, n_{k+1}-1}, \\ \Psi^{(k)} &= \Lambda_{n_{k+1}-l} V^{(k)}, & \text{where } V^{(k)} &:= [v_{ij}]_{i=0, \dots, n_{k+1}-l; j=n_k, \dots, n_{k+1}-1}, \end{aligned} \quad (5.19)$$

if  $0 \leq k \leq l-1$ , and

$$\begin{aligned} \Phi^{(l)} &= \Lambda_n U^{(l)}, & \text{where } U^{(l)} &:= [u_{ij}]_{i=0, \dots, n; j=n_l, \dots, n}, \\ \Psi^{(l)} &= \Lambda_n V^{(l)}, & \text{where } V^{(l)} &:= [v_{ij}]_{i=0, \dots, n; j=n_l, \dots, n}, \end{aligned} \quad (5.20)$$

if  $k = l$ . Note that, by (5.14), (5.17), and (5.20), we have

$$D^{(l)} = (V^{(l)})^T T_n U^{(l)}. \quad (5.21)$$

### 5.3. Further Properties

In this subsection, we collect some further properties of Algorithm 5.1 that will be needed later on.

Using (5.20), (4.13), (5.3), and the definition of  $\langle \cdot, \cdot \rangle$  in (3.1), one readily verifies that

$$T_n U^{(l)} = \begin{bmatrix} 0_{n_l \times h_l} \\ F^{(l)} \end{bmatrix}, \quad (V^{(l)})^T T_n = \begin{bmatrix} 0_{h_l \times n_l} & g^{(l)} \end{bmatrix}. \quad (5.22)$$

Next, we partition the matrices  $U^{(l)}$  and  $V^{(l)}$  in the form

$$U^{(l)} = \begin{bmatrix} \hat{U}^{(l)} \\ \tilde{U}^{(l)} \end{bmatrix}, \quad V^{(l)} = \begin{bmatrix} \hat{V}^{(l)} \\ \tilde{V}^{(l)} \end{bmatrix}, \quad \text{where } \tilde{U}^{(l)}, \tilde{V}^{(l)} \in \mathbb{C}^{h_l \times h_l}. \quad (5.23)$$

Note that  $\tilde{U}^{(l)}$  and  $\tilde{V}^{(l)}$  are unit upper triangular matrices, and in particular, they are nonsingular. With (5.21) and (5.23), it follows from (5.22) that

$$F^{(l)} = (\tilde{V}^{(l)})^{-T} D^{(l)}, \quad G^{(l)} = D^{(l)} (\tilde{U}^{(l)})^{-1}. \quad (5.24)$$

By means of the relations (5.24),  $F^{(l)}$  and  $G^{(l)}$  can be obtained without evaluating the bilinear forms  $\langle \Lambda^{(l)}, \Phi^{(l)} \rangle$  and  $\langle \Psi^{(l)}, \Lambda^{(l)} \rangle$  in step (5) of Algorithm 5.1, provided that  $D^{(l)}$  is available. It turns out that the elements of  $D^{(l)}$  can easily be updated from step to step; see Lemma 5.2 below.

Recall that the recurrence coefficients  $\xi_i^{(n)}$  and  $\zeta_i^{(n)}$  in (5.7) and (5.8), respectively, are still arbitrary. From now on, we assume that they are chosen as

$$\xi_i^{(n)} = \zeta_i^{(n)} = 0 \quad \text{for all } i, n. \quad (5.25)$$

Furthermore, it will be convenient to set

$$\alpha_k^{(1)} := (G^{(k)})^{-T} \begin{bmatrix} 0_{h_k-1} \\ 1 \end{bmatrix}, \quad \beta_k^{(1)} := (F^{(k)})^{-1} \begin{bmatrix} 0_{h_k-1} \\ 1 \end{bmatrix}. \quad (5.26)$$

Note that, with (5.26), the coefficient vectors  $\alpha_n, \beta_n$  in step (3) and step (4) of Algorithm 5.1 are given by

$$\alpha_n = \rho_n \alpha_l^{(1)}, \quad \beta_n = \tau_n \beta_l^{(1)} \quad \text{and} \quad \alpha_n = \rho_n \alpha_{l-1}^{(1)}, \quad \beta_n = \tau_n \beta_{l-1}^{(1)}, \quad (5.27)$$

respectively.

By (5.12) and (5.2), the matrix  $D^{(l)}$  is given by

$$D^{(l)} = [\langle \psi_i, \varphi_j \rangle]_{i,j=n_l, \dots, n}. \quad (5.28)$$

In the following lemma, we give formulas for updating the elements of (5.28) in the course of Algorithm 5.1.

LEMMA 5.2. *Let  $\varphi_{n+1}, \psi_{n+1}$  be the polynomials constructed in step  $n$  of Algorithm 5.1.*

(a) *If  $\varphi_{n+1}, \psi_{n+1}$  are constructed as regular FBOPs, then*

$$\begin{aligned} \langle \psi_{n+1}, \varphi_{n+1} \rangle &= \langle \psi_n, \varphi_n \rangle - \rho_n \begin{bmatrix} \tau_n & 0 & g_l^T \end{bmatrix} J V^{(l)} \alpha_l^{(1)} \\ &\quad - \begin{bmatrix} \tau_n & 0 & g_l^T \end{bmatrix} U^{(l)} \mu_n. \end{aligned} \quad (5.29)$$

(b) *If  $\varphi_{n+1}, \psi_{n+1}$  are constructed as inner polynomials, then*

$$\langle \psi_{m+1}, \varphi_{n+1} \rangle = \begin{cases} v_{0, n_l} \rho_n & \text{if } m+1 = n_l, \\ \langle \psi_m, \varphi_n \rangle + v_{0, m+1} \rho_n & \text{if } n_l < m+1 \leq n+1, \end{cases} \quad (5.30)$$

and

$$\langle \psi_{n+1}, \varphi_{m+1} \rangle = \begin{cases} u_{0, n_l} \tau_n & \text{if } m+1 = n_l, \\ \langle \psi_n, \varphi_m \rangle + u_{0, m+1} \tau_n & \text{if } n_l < m+1 \leq n+1. \end{cases} \quad (5.31)$$

*Proof.* First we show part (a). Here the polynomials  $\psi_{n+1}$  and  $\varphi_{n+1}$  are given by (5.6) and (5.5), respectively. Using (5.6), the biorthogonality conditions (4.13), (5.5), (3.3), and the first formula for  $\alpha_n$  in (5.27), one readily verifies that

$$\begin{aligned} \langle \psi_{n+1}, \varphi_{n+1} \rangle &= \langle \lambda \psi_n - \hat{\Phi}^{(l)} \beta_n - \Psi^{(l)} \nu_n, \varphi_{n+1} \rangle \\ &= \langle \lambda \psi_n, \varphi_{n+1} \rangle = \langle \lambda \psi_n, \lambda \varphi_n - \hat{\Psi}^{(l)} \alpha_n - \Phi^{(l)} \mu_n \rangle \\ &= \langle \psi_n, \varphi_n \rangle - \rho_n \langle \lambda \psi_n, \hat{\Psi}^{(l)} \alpha_l^{(1)} \rangle - \langle \lambda \psi_n, \Phi^{(l)} \rangle \mu_n. \end{aligned} \quad (5.32)$$



In view of (4.31) and (4.32), we have

$$\langle \lambda \psi_n, \Lambda_n \rangle = \begin{bmatrix} \tau_n & 0 & g_l^T \end{bmatrix}. \quad (5.33)$$

Note that, by (5.20) and (2.7),  $\Phi^{(l)} = \Lambda_n U^{(l)}$  and  $\hat{\Psi}^{(l)} = \Lambda_n J V^{(l)}$ . In view of (5.33), it follows that

$$\begin{aligned} \langle \lambda \psi_n, \hat{\Psi}^{(l)} \rangle &= \begin{bmatrix} \tau_n & 0 & g_l^T \end{bmatrix} J V^{(l)}, \\ \langle \lambda \psi_n, \Phi^{(l)} \rangle &= \begin{bmatrix} \tau_n & 0 & g_l^T \end{bmatrix} U^{(l)}. \end{aligned} \quad (5.34)$$

By inserting (5.34) into (5.32), we obtain the relation (5.29).

Now we turn to part (b). Since the proofs of (5.30) and (5.31) are completely analogous, we will only show (5.30). We assume that  $\varphi_{n+1}$  is constructed as an inner polynomial; note that  $\varphi_{n+1}$  is given by (5.7), where, by (5.25),  $\xi_i^{(n)} = 0$  for all  $i$ . Let  $n_l \leq m+1 \leq n+1$ . From (5.6) if  $m+1 = n_l$ , and (5.8) (with  $\zeta_i^{(m)} = 0$  for all  $i$ ) if  $m+1 > n_l$ , it follows that  $\psi_{m+1}$  can be written in the form

$$\psi_{m+1}(\lambda) \equiv \psi_{m+1}(0) + \lambda \psi_m(\lambda) + \lambda \chi_m(\lambda) \quad \text{for some } \chi_m \in \mathcal{P}_{n_l-2}. \quad (5.35)$$

Moreover, in view of the representation (5.13) of  $\psi_{m+1}$ , we have

$$\psi_{m+1}(0) = v_{0, m+1}. \quad (5.36)$$

Using (5.7), (4.13), (5.35), (3.3), (5.36), and the formula for  $\rho_n$  in (5.4), one easily verifies that

$$\begin{aligned} \langle \psi_{m+1}, \varphi_{n+1} \rangle &= \langle \psi_{m+1}, \lambda \varphi_n - \hat{\Psi}^{(l-1)} \alpha_n \rangle = \langle \psi_{m+1}, \lambda \varphi_n \rangle \\ &= \psi_{m+1}(0) \langle 1, \lambda \varphi_n \rangle + \langle \lambda \psi_m, \lambda \varphi_n \rangle + \langle \lambda \chi_m, \lambda \varphi_n \rangle \\ &= v_{0, m+1} \rho_n + \langle \psi_m, \varphi_n \rangle. \end{aligned} \quad (5.37)$$

If  $m+1 > n_l$ , then (5.37) is just the desired relation (5.30). If  $m+1 = n_l$ ,

then, by (4.13) and since  $n \geq n_l > m$ , we have  $\langle \psi_m, \varphi_n \rangle = 0$ , and thus (5.37) reduces to (5.30).  $\blacksquare$

Typically, Algorithm 5.1 will perform mostly regular steps (3), and then the formulas (5.5) and (5.6) simplify somewhat. Indeed, assume that Algorithm 5.1 performs regular steps in two consecutive iterations, i.e.,

$$n + 1 = n_{l+1} = n_l + 1 \quad \text{and} \quad h_l = n_{l+1} - n_l = 1. \quad (5.38)$$

Using (5.3), (5.2), (4.13), and (5.12), one easily shows that, in this case,

$$F^{(l)} = G^{(l)} = \langle \psi_n, \varphi_n \rangle = D^{(l)}. \quad (5.39)$$

With (5.39), (4.16), (5.5), and (5.6), we conclude that

$$f_l = g_l = \emptyset, \quad \mu_n = \nu_n = 0, \quad \alpha_n = \frac{\rho_n}{\langle \psi_n, \varphi_n \rangle}, \quad \beta_n = \frac{\tau_n}{\langle \psi_n, \varphi_n \rangle}. \quad (5.40)$$

In particular, the recurrences for  $\varphi_{n+1}$  and  $\psi_{n+1}$  in (5.5) and (5.6) reduce to

$$\varphi_{n+1} = \lambda \varphi_n - \hat{\psi}_n \alpha_n \quad \text{and} \quad \psi_{n+1} = \lambda \psi_n - \hat{\varphi}_n \beta_n, \quad (5.41)$$

respectively. Furthermore, with (5.40), (5.26), (5.39), and since  $JV^{(l)} = Jv_n = [1 \ \cdots]^T$ , it follows that the update formula (5.29) reduces to

$$\langle \psi_{n+1}, \varphi_{n+1} \rangle = \langle \psi_n, \varphi_n \rangle \left( 1 - \frac{\rho_n \tau_n}{\langle \psi_n, \varphi_n \rangle^2} \right). \quad (5.42)$$

Note that, in view of (4.4), the recursions (5.41) and (5.42) are identical to the update formulas (4.2) and (4.3). In other words, the  $n$ th step of Algorithm 5.1 just reduces to the  $n$ th step of the Szegő Algorithm 4.1, if (5.38) is satisfied. In particular, for the case that  $n_{k+1} = n_k + 1$  for all  $k = 0, 1, \dots$ , we have the following result.

**COROLLARY 5.3.** *If all polynomials are constructed as regular FBOPs, then Algorithm 5.1 reduces to the Szegő Algorithm 4.1.*

## 6. A LOOK-AHEAD TOEPLITZ-SYSTEM SOLVER

In this section, we present our look-ahead Levinson algorithm for solving general Toeplitz systems. We give implementation details and operation counts, and we describe the look-ahead strategy.

### 6.1. The Algorithm

By means of (5.13), Algorithm 5.1 can be rewritten in terms of the coefficient vectors  $u_n$  and  $v_n$  of the polynomials  $\varphi_n$  and  $\psi_n$ ,  $n = 0, 1, \dots$ . Recall from Section 5.2 that these vectors are just the columns of the triangular matrices  $U_n$  and  $V_n$  in the factorization (5.14)–(5.17) of  $T_n$ . We call  $u_n$  and  $v_n$  *regular vectors* if they are the coefficient vectors of regular FBOPs  $\varphi_n$  and  $\psi_n$ , and *inner vectors* if they correspond to a pair of inner polynomials.

In the following, we denote by  $s_n, r_n \in \mathbb{C}^{n+1}$  the vectors defined by the partitioning

$$T_{n+1} = \begin{bmatrix} t_0 & s_n^T \\ r_n & T_n \end{bmatrix} \quad (6.1)$$

of  $T_{n+1}$ . In view of (5.13), we have

$$\lambda \varphi_n = \Lambda_{n+1} \begin{bmatrix} 0 \\ u_n \end{bmatrix} \quad \text{and} \quad \lambda \psi_n = \Lambda_{n+1} \begin{bmatrix} 0 \\ v_n \end{bmatrix}. \quad (6.2)$$

From (6.1), (6.2), and the definition of  $\langle \cdot, \cdot \rangle$  in (3.1), it follows that

$$\langle 1, \lambda \varphi_n \rangle = s_n^T u_n \quad \text{and} \quad \langle \lambda \psi_n, 1 \rangle = v_n^T r_n. \quad (6.3)$$

Also, note that  $\langle 1, 1 \rangle = t_0$ . Finally, using (5.13), (6.3), (5.19), (5.20), (2.7), (5.25), and the vectors  $\alpha_k^{(1)}, \beta_k^{(1)}$  defined in (5.26), we can rewrite Algorithm 5.1 as follows.

**ALGORITHM 6.1** (Inverse block-factorization of general  $T_n$ ).

(0) Set  $u_0 = v_0 = 1$ ,  $U^{(0)} = V^{(0)} = 1$ ,  $F^{(0)} = G^{(0)} = t_0$ ,  $n_0 = 0$ ,  $l = 0$ .

For  $n = 0, 1, \dots$ , do:

(1) Compute

$$\rho_n = s_n^T u_n, \quad \tau_n = v_n^T r_n. \quad (6.4)$$

(2) Decide whether to construct  $u_{n+1}$  and  $v_{n+1}$  as regular vectors or as inner vectors, and go to (3) or (4), respectively.

(3) (Regular step.) Compute  $\alpha_l^{(1)}$ ,  $\mu_n$ ,  $\beta_l^{(1)}$ ,  $\nu_n$  by solving

$$\begin{aligned} (G^{(l)})^T \alpha_l^{(1)} &= \begin{bmatrix} 0 \\ 1 \end{bmatrix}, & F^{(l)} \mu_n &= \begin{bmatrix} 0 \\ f_l \end{bmatrix}, & F^{(l)} \beta_l^{(1)} &= \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \\ (G^{(l)})^T \nu_n &= \begin{bmatrix} 0 \\ g_l \end{bmatrix}, \end{aligned} \quad (6.5)$$

respectively, and set

$$\begin{aligned} u_{n+1} &= \begin{bmatrix} 0 \\ u_n \end{bmatrix} - \rho_n \begin{bmatrix} JV^{(l)} \\ 0 \end{bmatrix} \alpha_l^{(1)} - \begin{bmatrix} U^{(l)} \\ 0 \end{bmatrix} \mu_n, \\ v_{n+1} &= \begin{bmatrix} 0 \\ v_n \end{bmatrix} - \tau_n \begin{bmatrix} JU^{(l)} \\ 0 \end{bmatrix} \beta_l^{(1)} - \begin{bmatrix} V^{(l)} \\ 0 \end{bmatrix} \nu_n. \end{aligned} \quad (6.6)$$

Set  $n_{l+1} = n + 1$ ,  $l = l + 1$ ,  $U^{(l)} = V^{(l)} = F^{(l)} = G^{(l)} = \emptyset$ , and go to (5).

(4) (Inner step.) Set

$$u_{n+1} = \begin{bmatrix} 0 \\ u_n \end{bmatrix} - \rho_n \begin{bmatrix} JV^{(l-1)} \\ 0 \end{bmatrix} \alpha_{l-1}^{(1)}, \quad v_{n+1} = \begin{bmatrix} 0 \\ v_n \end{bmatrix} - \tau_n \begin{bmatrix} JU^{(l-1)} \\ 0 \end{bmatrix} \beta_{l-1}^{(1)}.$$

(5) Set

$$U^{(l)} = \left[ \begin{array}{c|c} U^{(l)} & u_{n+1} \end{array} \right], \quad V^{(l)} = \left[ \begin{array}{c|c} V^{(l)} & v_{n+1} \end{array} \right],$$

and update  $F^{(l)}$ ,  $G^{(l)}$ .

Note that Algorithm 6.1 only computes the inverse block-factorization (5.14) of  $T_n$ . Next, we discuss how to obtain solutions for nested Toeplitz

systems

$$T_n x_n = b_n, \quad n = 0, 1, \dots \quad (6.7)$$

Here the right-hand sides  $b_n \in \mathbb{C}^{n+1}$  are assumed to be nested, i.e.,

$$b_{n+1} = \begin{bmatrix} b_n \\ \sigma_{n+1} \end{bmatrix}, \quad \text{with } \sigma_{n+1} \in \mathbb{C}, \quad \text{for all } n.$$

Recall that  $T_n$  is guaranteed to be nonsingular for  $n = n_k - 1, k = 1, 2, \dots, l$ , and we only update the solution  $x_n$  of (6.7) for these values of  $n$ . To this end, we simply need to insert the following procedure at the beginning of each regular step (3) in Algorithm 6.1:

Set  $n' = n_l - 1$ , and partition  $b_n$  and  $T_n$  as follows:

$$b_n = \begin{bmatrix} b_{n'} \\ \sigma \end{bmatrix}, \quad T_n = \begin{bmatrix} T_{n'} & S \\ R & T_{n-n'} \end{bmatrix}, \quad (6.8)$$

where  $\sigma$  just contains the last  $n - n'$  elements of  $b_n$ . Compute  $y$  by solving

$$F^{(l)} y = \sigma - R x_{n'}, \quad (6.9)$$

and set

$$x_n = \begin{bmatrix} x_{n'} \\ 0_{n-n'} \end{bmatrix} + U^{(l)} y. \quad (6.10)$$

We need to show that  $x_n$  given by (6.10) and (6.9) is the solution of (6.7). Indeed, by means of (6.8)–(6.10) and the first relation in (5.22), it follows that

$$T_n x_n = \begin{bmatrix} T_{n'} \\ R \end{bmatrix} x_{n'} + T_n U^{(l)} y = \begin{bmatrix} b_{n'} \\ R x_{n'} \end{bmatrix} + \begin{bmatrix} 0 \\ F^{(l)} \end{bmatrix} (F^{(l)})^{-1} (\sigma - R x_{n'}) = b_n.$$

## 6.2. Implementation Details and Operation Counts

We now discuss some implementation details for Algorithm 6.1, and we present operation counts.

Except for contrived examples, Toeplitz matrices that arise in practical applications have at most a small number of consecutive ill-conditioned leading principal submatrices. Consequently, Algorithm 6.1 mostly performs regular steps. Typically, only a few true look-ahead steps occur, and their length  $h_l$  is usually small, mostly  $h_l = 2$ . Actually, as we will discuss in detail in Section 6.3 below, the only parameter that the user needs to provide is an upper bound, called  $h_{\max}$ , for the maximal length  $h_l$  of a look-ahead step. If no information on the number of consecutive ill-conditioned leading principal submatrices is available, then we recommend to set  $h_{\max} = 5$ . This justifies the following convention that we will use for the operation count: a computation that requires only arithmetic operations of order  $O(h_l^3)$  or less is considered *negligible*.

We now consider steps (1)–(5) of Algorithm 6.1 in more detail. Step (1) involves the computation of two inner products of vectors of length  $n + 1$ . It turns out that these are the only two inner products that are required during the  $n$ th iteration. This is exactly the same as in the classical Levinson algorithm for strongly regular matrices.

The look-ahead strategy for the decision in step (2) will be described in Section 6.3. As we will see there, it only involves negligible work.

Next we turn to step (3). Note that  $(G^{(l)})^T$  and  $F^{(l)}$  are  $h_l \times h_l$  matrices; if  $h_l > 1$ , we use Gaussian elimination to solve the four linear systems in (6.5). Recall from (4.17) that  $f_l$  and  $g_l$  are given as part of the last columns of  $F^{(l)}$  and  $(G^{(l)})^T$ . If  $h_l = 1$ , then, by (5.40),  $\mu_n = \nu_n = 0$ , and the two updates in (6.6) require two SAXPYS<sup>2</sup> with vectors of length  $n + 1$ . If  $h_l > 1$ , then we first compute the two vectors

$$JV^{(l)}\alpha_l^{(1)} \quad \text{and} \quad JU^{(l)}\beta_l^{(1)}, \quad (6.11)$$

which costs  $2h_l$  SAXPYS. The two updates in (6.6) then require  $2(h_l + 1)$  additional SAXPYS.

Step (4) always requires two SAXPYS. This is obvious if  $h_{l-1} = 1$ . If  $h_{l-1} > 1$ , we use the vectors (6.11) (with  $l$  replaced by  $l - 1$ ), which were already computed in the course of the last regular step.

In step (5), we need to update the matrices  $F^{(l)}$  and  $G^{(l)}$ . To this end, we first update  $D^{(l)}$  using Lemma 5.2, and then we compute  $F^{(l)}$  and  $G^{(l)}$  by means of (5.24). Note that, by (5.23), the triangular matrices  $\tilde{U}^{(l)}$  and  $\tilde{V}^{(l)}$  in (5.24) are given as part of  $U^{(l)}$  and  $V^{(l)}$ . Consequently, step (5) only involves negligible work.

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<sup>2</sup>A SAXPY operation is  $z = x + \alpha y$ , where  $x$  and  $y$  are vectors and  $\alpha$  is a scalar; see, e.g., [17].

Finally, we turn to the procedure for updating solutions of Toeplitz systems (6.7). To compute the right-hand side of (6.9), we need to generate  $Rx'_n$ , which involves  $h_l = n - n'$  inner products. The computation of the vector  $x_n$  in (6.10) requires another  $h_l$  SAXPYS. Note that  $x_n$  is only updated once within each cycle of  $h_l$  steps. Thus, in the average, the update procedure requires one inner product and one SAXPY per  $n$ th step.

In Table 1, we summarize the operation counts for one step of Algorithm 6.1, and for the updating procedure for solutions of general Toeplitz systems (6.7).

### 6.3. The Look-Ahead Strategy

The look-ahead strategy is crucial both for the accuracy and the efficiency of Algorithm 6.1. Its main purpose is to skip over ill-conditioned leading principal submatrices in order to avoid breakdowns and numerical instabilities. However, as is obvious from the operation counts in Table 1, it is more expensive to perform a look-ahead step of length  $h_l > 1$  than  $h_l$  classical Levinson steps. Therefore, for the sake of efficiency, it is desirable to perform look-ahead steps only when necessary. The look-ahead strategy is implemented through the criteria that are used in step (2) of Algorithm 6.1 to decide whether the next vectors are constructed as regular or inner ones. There are two quantities, denoted by  $\kappa(\Gamma^{(l)})$  and  $\eta_n$ , that are monitored throughout the algorithm. Both of them are obtained from local information only. In particular, we do not need to estimate the condition number of the current leading principal submatrix  $T_n$ . The decision about building regular or inner vectors is then based on a comparison of  $\kappa(\Gamma^{(l)})$  and  $\eta_n$  with two threshold parameters COND ( $> 0$ ) and GFACTOR ( $\geq 1$ ), respectively. The algorithm dynamically determines COND and GFACTOR, and the only input that is required from the user is the number  $h_{\max}$ , which is the maximal length of a look-ahead step the algorithm is allowed to perform. Note that, in view of (5.18), we then have

$$h_k \leq h_{\max} \quad \text{for all } k,$$

TABLE 1  
OPERATION COUNTS FOR ALGORITHM 6.1

	Regular step		Inner step	Update of $x_n$
	With $h_l = 1$	With $h_l > 1$		
Inner products/step	2	2	2	1
SAXPYS/step	2	$2(2h_l + 1)$	2	1

and Algorithm 6.1 generates an inverse block-factorization (5.14) with blocks of size  $\leq h_{\max}$ . We remark that Algorithm 6.1 reduces to the classical Levinson algorithm if we set  $h_{\max} = 1$ .

The initialization phase of the algorithm is as follows. As the first block, we set  $D^{(0)} = T_m$ , where  $T_m$  is the matrix with the smallest condition number<sup>3</sup>  $\kappa(T_m)$  among  $T_h$ ,  $h = 0, 1, \dots, h_{\max} - 1$ . Then we build the next vectors  $u_{m+1}$  and  $v_{m+1}$  as regular vectors, and we set  $n_1 = m + 1$ . Furthermore, we initialize COND to be this smallest condition number  $\kappa(T_m)$ , and we set GFACTOR to 1.

Now we consider a general iteration step of Algorithm 6.1. As we mentioned before, for the sake of efficiency, the look-ahead Toeplitz solver should build as many regular vectors as possible. Therefore, in each iteration step, we first pretend that  $u_{n+1}$  and  $v_{n+1}$  can actually be constructed as regular vectors. Recall from (5.9) that, for a regular step, it is necessary that  $F^{(l)}$  and  $G^{(l)}$  are nonsingular. To check this condition, we compute the matrix

$$\Gamma^{(l)} := (\tilde{V}^{(l)})^{-T} D^{(l)} (\tilde{U}^{(l)})^{-1},$$

where  $\tilde{U}^{(l)}$  and  $\tilde{V}^{(l)}$  are the triangular matrices given by (5.23). Note that, by (5.24), we have

$$\Gamma^{(l)} = F^{(l)} (\tilde{U}^{(l)})^{-1} = (\tilde{V}^{(l)})^{-T} G^{(l)},$$

and hence  $F^{(l)}$  and  $G^{(l)}$  are nonsingular if, and only if,  $\Gamma^{(l)}$  is nonsingular. We now check whether

$$\kappa(\Gamma^{(l)}) \leq 2 \times \text{COND}. \quad (6.12)$$

If (6.12) is not satisfied, then we go to step (4) in Algorithm 6.1, and we build  $u_{n+1}$  and  $v_{n+1}$  as inner vectors. To justify the criterion (6.12), recall that, in view of Lemma 3.1,  $T_n$  is required to be nonsingular for a regular step. Actually, at the end of this section, we will point out that  $\kappa(\Gamma^{(l)})$  is closely related to  $\kappa(T_n)$ .

If (6.12) is satisfied, then we compute the quantities  $\alpha_n$ ,  $\mu_n$ ,  $\beta_n$ , and  $\nu_n$ , using (6.5) and the first two relations in (5.27), and we set

$$\eta_n := \max\{\|\alpha_n\|_1, \|\mu_n\|_1, \|\beta_n\|_1, \|\nu_n\|_1\}.$$

---

<sup>3</sup>Recall the definition of  $\kappa$  in (2.1).



Here  $\|x\|_1 := |\xi_1| + \cdots + |\xi_h|$  denotes the 1-norm of a vector  $x = [\xi_1 \ \cdots \ \xi_h]^T \in \mathbb{C}^h$ . Then, we check whether

$$\eta_n \leq 2 \times \text{GFACTOR}. \quad (6.13)$$

If the criterion (6.13) is not satisfied, we proceed with step (4) and construct  $u_{n+1}$  and  $v_{n+1}$  as inner vectors. The justification for (6.13) is as follows. Note that, by (5.14),

$$T_{n+1} = V_{n+1}^{-T} D_{n+1} U_{n+1}^{-1} \quad \text{and} \quad T_{n+1}^T = U_{n+1}^{-T} D_{n+1}^T V_{n+1}^{-1}. \quad (6.14)$$

If one computed the decompositions (6.14) of  $T_{n+1}$  or  $T_{n+1}^T$  directly by means of Gaussian elimination, then pivoting would be used to ensure that the size of the off-diagonal elements of  $U_{n+1}^{-1}$  and  $V_{n+1}^{-1}$  was bounded by 1. Indeed, this is the key to numerical stability of Gaussian elimination. Recall that the elements of the strictly upper triangular parts of  $U_{n+1}^{-1}$  and  $V_{n+1}^{-1}$  are just the multipliers in Gaussian elimination. Now, for Toeplitz matrices pivoting would destroy the Toeplitz structure. Roughly speaking, the look-ahead Algorithm 6.1 performs a true look-ahead step of length  $h_l > 1$  whenever one would encounter a small pivot in Gaussian elimination. Consequently, the look-ahead strategy should also guarantee that off-diagonal elements of  $U_{n+1}^{-1}$  and  $V_{n+1}^{-1}$  are not too large. Since

$$U_{n+1}^{-1} = I + C + C^2 + \cdots + C^{n+1}, \quad \text{where} \quad C := I - U_{n+1},$$

a large off-diagonal element of  $U_{n+1}$  usually leads to a large off-diagonal element of  $U_{n+1}^{-1}$ . A similar conclusion also holds for  $V_{n+1}^{-1}$ . Therefore, in each step of the Algorithm 6.1, we limit the growth in the newly generated off-diagonal elements of  $U_{n+1}$  and  $V_{n+1}$ , which are just the components of  $u_{n+1}$  and  $v_{n+1}$ . This is the purpose of imposing the check (6.13).

If both criteria (6.12) and (6.13) are satisfied, then we proceed with step (3) in Algorithm 6.1 and construct  $u_{n+1}$  and  $v_{n+1}$  as regular vectors.

It cannot be excluded that the algorithm has reached the maximal block size  $h_{\max}$ , but the two checks for building the next vectors as regular ones are still not satisfied. More precisely, the algorithm has built a pair of blocks  $U^{(l)}$  and  $V^{(l)}$  of size  $h_{\max}$ , both starting with index  $n_l$  and ending with index  $n_l + h_{\max} - 1$ , and the criteria (6.12) and (6.13) for constructing  $u_{n_l+h_{\max}}$  and  $v_{n_l+h_{\max}}$  as regular vectors are not fulfilled. In this case, we adjust the values of the threshold parameters COND and GFACTOR in such a way that the criteria for building regular vectors are satisfied within the maximal look-ahead

size  $h_{\max}$ . To this end, we first determine a step size  $h \in \{1, 2, \dots, h_{\max}\}$  such that

$$\kappa(\Gamma_h^{(l)}) + |\Gamma_1^{(l)}| \eta_{n_l+h-1} \quad (6.15)$$

is minimal. Here  $\Gamma_j^{(l)}$ ,  $j = 1, \dots, h_{\max}$ , denotes the  $j \times j$  leading principal submatrix of  $\Gamma^{(l)}$ . We then set COND to the condition number of the corresponding  $\Gamma_h^{(l)}$ , and the second parameter GFACOR to the value of the corresponding  $\eta_{n_l+h-1}$ . This choice of  $h$  guarantees that the vectors with index  $n_l + h$  can be constructed as regular vectors. The motivation for the choice (6.15) is as follows. From the above discussion, it is clear that the goal is to minimize simultaneously  $\kappa(\Gamma_h^{(l)})$  and  $\eta_{n_l+h-1}$ ; this is exactly what (6.15) attempts to ensure. The weighting factor  $|\Gamma_1^{(l)}|$  in (6.15) was chosen based on extensive numerical tests, and the choice (6.15) was found to work satisfactorily in practice. With the described look-ahead strategy, the algorithm can be expected to produce accurate solutions of Toeplitz systems as long as the coefficient matrix has at most  $h_{\max} - 1$  consecutive ill-conditioned leading principal submatrices.

We conclude this section with a discussion of the connection of the condition numbers of  $\Gamma^{(l)}$  and  $T_n$ . We set  $n' := n_l - 1$ , and we partition  $T_n$  as follows:

$$T_n = \begin{bmatrix} T_{n'} & S \\ R & \tilde{T} \end{bmatrix}.$$

Here  $T_{n'}$  is the last well-conditioned Toeplitz submatrix. With this notation,  $\Gamma^{(l)}$  is, in fact, the Schur complement of  $T_{n'}$  in  $T_n$ , and we have the decomposition

$$T_n = \begin{bmatrix} I & 0 \\ RT_{n'}^{-1} & I \end{bmatrix} \begin{bmatrix} T_{n'} & 0 \\ 0 & \Gamma^{(l)} \end{bmatrix} \begin{bmatrix} I & T_{n'}^{-1}S \\ 0 & I \end{bmatrix},$$

which implies that

$$\begin{aligned} \Gamma^{(l)} &= \begin{bmatrix} 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ -RT_{n'}^{-1} & I \end{bmatrix} T_n \begin{bmatrix} I & -T_{n'}^{-1}S \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 \\ I \end{bmatrix} \\ &= \begin{bmatrix} -RT_{n'}^{-1} & I \end{bmatrix} T_n \begin{bmatrix} -T_{n'}^{-1}S \\ I \end{bmatrix}. \end{aligned} \quad (6.16)$$

From (6.16), it follows that

$$\|\Gamma^{(l)}\| \leq \left\| \begin{bmatrix} -RT_{n'}^{-1} & I \end{bmatrix} \right\| \cdot \left\| \begin{bmatrix} -T_{n'}^{-1}S \\ I \end{bmatrix} \right\| \cdot \|T_n\|.$$

It can be verified that

$$\left\| \begin{bmatrix} -RT_{n'}^{-1} & I \end{bmatrix} \right\| \leq \sqrt{1 + \left( \frac{\|R\| \kappa(T_{n'})}{\|T_{n'}\|} \right)^2},$$

$$\left\| \begin{bmatrix} -T_{n'}^{-1}S \\ I \end{bmatrix} \right\| \leq \sqrt{1 + \left( \frac{\|S\| \kappa(T_{n'})}{\|T_{n'}\|} \right)^2}.$$

Therefore, setting

$$\varrho := \sqrt{1 + \left( \frac{\|R\| \kappa(T_{n'})}{\|T_{n'}\|} \right)^2} \sqrt{1 + \left( \frac{\|S\| \kappa(T_{n'})}{\|T_{n'}\|} \right)^2},$$

we have

$$\|\Gamma^{(l)}\| \leq \varrho \|T_n\|. \quad (6.17)$$

Similarly, we can show

$$\|(\Gamma^{(l)})^{-1}\| \leq \varrho \|T_n^{-1}\|. \quad (6.18)$$

To get bounds for the condition numbers, we distinguish two cases. First, assume that  $\Gamma^{(l)}$  is of size  $> 1$ . Then, by combining (6.17) and (6.18), we arrive at

$$\kappa(T_n) \leq \varrho^2 \kappa(\Gamma^{(l)}).$$

With the same technique, we can show that

$$\kappa(\Gamma^{(l)}) \leq \varrho^2 \kappa(T_n),$$

and hence

$$\kappa(T_n)/\varrho^2 \leq \kappa(\Gamma^{(l)}) \leq \varrho^2 \kappa(T_n). \quad (6.19)$$

For the case that  $\Gamma^{(l)}$  is a scalar, from (6.17) and (6.18), we obtain

$$\frac{1}{\varrho \|T_n\|} \leq \kappa(\Gamma^{(l)}) \leq \varrho \|T_n^{-1}\|. \quad (6.20)$$

Roughly speaking, the inequalities (6.19) and (6.20) state that if  $T_{n'}$  is well conditioned, then  $T_n$  is well conditioned if, and only if,  $\Gamma^{(l)}$  is well conditioned.

## 7. THE SPECIAL CASE OF HERMITIAN TOEPLITZ MATRICES

In this section, we consider the special case of Hermitian Toeplitz matrices.

### 7.1. A Look-Ahead Levinson Algorithm

Suppose that the elements of the biinfinite sequence  $\{t_i\}_{i=-\infty}^{\infty}$  satisfy  $t_{-i} = \bar{t}_i$  for all  $i$ . Then the Toeplitz matrices (1.1) are all Hermitian, i.e.,

$$T_n = T_n^H, \quad n = 0, 1, \dots \quad (7.1)$$

Using (7.1) and the definition of  $\langle \cdot, \cdot \rangle$ , one easily verifies that regular FBOPs and inner quasi-FBOPs associated with the bilinear form  $\langle \cdot, \cdot \rangle$  are connected by

$$\psi_n = \bar{\varphi}_n. \quad (7.2)$$

Here  $\bar{\varphi}$  denotes the polynomial whose coefficients are just the complex conjugates of the coefficients of  $\varphi$ . In other words, the coefficient vectors  $u_n$  and  $v_n$  of  $\varphi_n$  and  $\psi_n$  satisfy

$$v_n = \bar{u}_n. \quad (7.3)$$

Consequently, for Hermitian Toeplitz matrices, Algorithm 6.1 simplifies, since we only need to update the vectors  $u_n$ . Furthermore, note that, in (6.1),

$s_n = \bar{r}_n$ , and in view of (7.3) and (6.4), we obtain

$$\tau_n = v_n^T r_n = u_n^H r_n = (r_n^H u_n)^H = \bar{\rho}_n. \quad (7.4)$$

In view of (7.2), the matrices (4.12) are now connected by

$$F^{(k)} = (G^{(k)})^H. \quad (7.5)$$

Finally, using (7.3)–(7.5) and setting

$$\gamma_k^{(1)} := \overline{\alpha_k^{(1)}} = (F^{(k)})^{-1} \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

we obtain from Algorithm 6.1 the following look-ahead Levinson algorithm for Hermitian Toeplitz matrices.

ALGORITHM 7.1 (Inverse block-factorization of Hermitian  $T_n$ ).

(0) Set  $u_0 = 1$ ,  $U^{(0)} = 1$ ,  $F^{(0)} = t_0$ ,  $n_0 = 0$ ,  $l = 0$ .

For  $n = 0, 1, \dots$ , do:

(1) Compute  $\tau_n = u_n^H r_n$ .

(2) Decide whether to construct  $u_{n+1}$  as a regular vector or as an inner vector, and go to (3) or (4), respectively.

(3) (Regular step.) Compute  $\gamma_l^{(1)}$ ,  $\mu_n$ , by solving

$$F^{(l)} \gamma_l^{(1)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad F^{(l)} \mu_n = \begin{bmatrix} 0 \\ f_k \end{bmatrix},$$

respectively, and set

$$u_{n+1} = \begin{bmatrix} 0 \\ u_n \end{bmatrix} - \tau_n \begin{bmatrix} J \bar{U}^{(l)} \\ 0 \end{bmatrix} \gamma_l^{(1)} - \begin{bmatrix} U^{(l)} \\ 0 \end{bmatrix} \mu_n.$$

Set  $n_{l+1} = n + 1$ ,  $l = l + 1$ ,  $U^{(l)} = \emptyset$ , and go to (5).

(4) (Inner step.) Set

$$u_{n+1} = \begin{bmatrix} 0 \\ u_n \end{bmatrix} - \tau_n \begin{bmatrix} J \bar{U}^{(l-1)} \\ 0 \end{bmatrix} \gamma_{l-1}^{(1)}.$$

(5) Set

$$U^{(l)} = \left[ \begin{array}{c|c} U^{(l)} & \\ \hline 0 & u_{n+1} \end{array} \right],$$

and update  $F^{(l)}$ .

## 7.2. A Counterexample

Chan and Hansen proposed a look-ahead Levinson procedure that is different from our algorithm. Their method was first presented for the special case of real symmetric Toeplitz matrices [8], and then extended to general nonsymmetric Toeplitz systems in [9]. The derivation of their algorithm is actually based on the assumption that only *isolated* look-ahead steps occur, which are preceded and followed by standard Levinson steps. However, in general it cannot be excluded that  $T_n$  has two or more *consecutive* blocks of singular or ill-conditioned leading principal submatrices, which then require two or more *consecutive* look-ahead steps. In both papers [8] and [9], this case is treated separately, and special recurrences are derived for handling two consecutive look-ahead steps; see [8, Theorem 3] and [9, Theorem 2]. However, the proposed approach involves division by the first component  $c_1$  of a coefficient vector  $c$ ; see [8, Equation (5.9)] and [9, Equation (50)]. Unfortunately, it is not guaranteed that  $c_1 \neq 0$ , and thus division by 0 can occur. Indeed, we now present a real symmetric Toeplitz matrix for which  $c_1 = 0$ . Consequently, the look-ahead Levinson algorithm proposed by Chan and Hansen can break down for general Toeplitz systems, as well as for the special case of Hermitian Toeplitz matrices.

Consider the  $7 \times 7$  Toeplitz matrix

$$T_6 = \begin{bmatrix} 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 \end{bmatrix}. \quad (7.6)$$

This matrix has exactly singular leading principal submatrices  $T_0$ ,  $T_2$ ,  $T_3$ , and  $T_4$ , while the remaining submatrices  $T_1$ ,  $T_5$ , and  $T_6$  are all nonsingular with condition numbers  $\kappa(T_1) = 1$ ,  $\kappa(T_5) \approx 18.1$ , and  $\kappa(T_6) \approx 7.2$ . In particular,  $T_1$  is optimally conditioned, and the algorithm in [8] starts with a look-ahead

step of length 2, followed by another look-ahead step of length 4 or 5. For the update of quantities corresponding to the second look-ahead step, the algorithm [8] requires division by the first component  $c_1$  of a vector  $c$  that, using the notation from [8], is given as follows:

$$r_4^{(2)} = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 1 \end{bmatrix}, \quad y_2 = -\begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad R_4 = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix},$$

$$c = -r_4^{(2)} - R_4^T J y_2 = \begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix}.$$

Thus we have  $c_1 = 0$ , and the algorithm breaks down in the course of the second look-ahead step.

## 8. NUMERICAL EXPERIMENTS

In this section, we report results of numerical experiments with the look-ahead Algorithms 6.1 and 7.1, and the classical Levinson algorithm. All computations were carried out using MATLAB on a DEC 3100 workstation with machine precision of order  $10^{-16}$ . For all the examples, we generated the right-hand side  $b_n$  such that the vector of all 1's is the exact solution  $x_{\text{exact}}$  of  $T_n x_n = b_n$ . In the following, we always list the relative error defined as

$$\text{relative error} = \frac{\|x_{\text{compt}} - x_{\text{exact}}\|}{\|x_{\text{exact}}\|},$$

where  $x_{\text{compt}}$  is the computed solution.

**EXAMPLE 1.** This test set consists of 100 nonsymmetric  $64 \times 64$  matrices with at least one ill-conditioned leading principal submatrix. The off-diagonal entries  $t_i$  of these matrices were generated as random numbers in  $[-1, 1]$ , and  $t_0$  was then chosen so that at least one submatrix is ill-conditioned. A typical condition-number profile of a matrix in this test set is shown in Figure 1. First, we use the classical Levinson algorithm, and in Figure 2, we show—in the form of a histogram—the relative errors for the 100 test

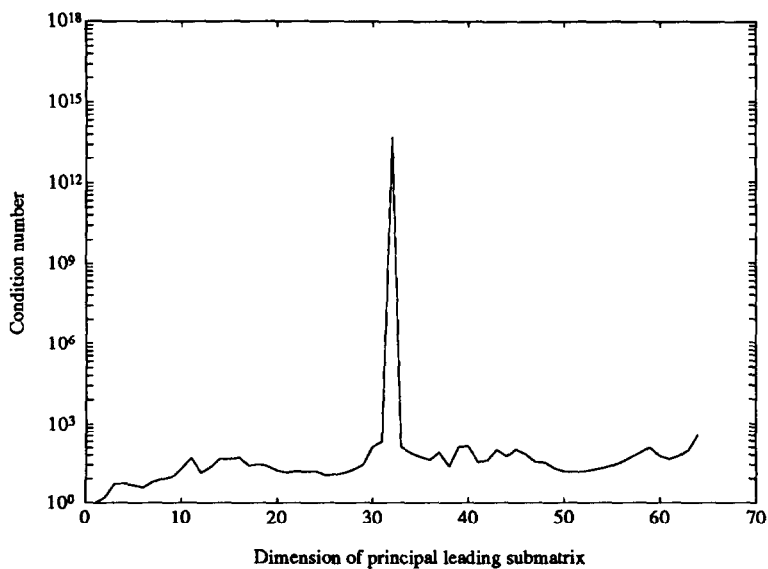
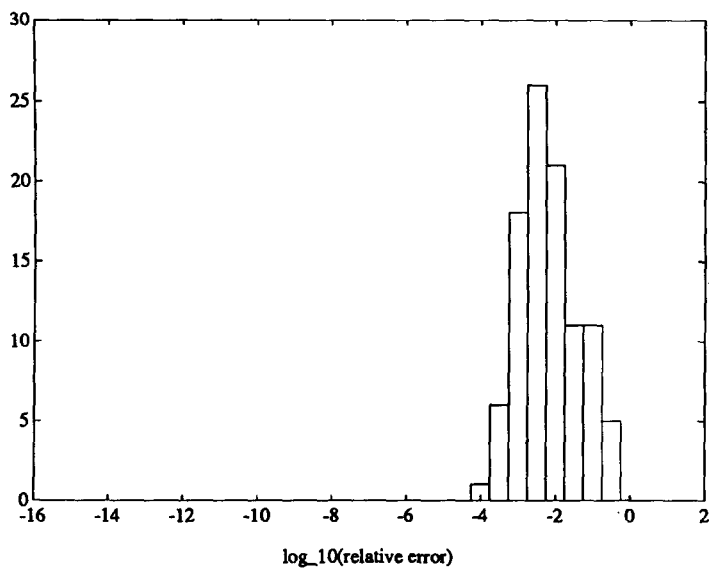
FIG. 1. Condition-number profile of a  $64 \times 64$  Toeplitz matrix.

FIG. 2. Histogram of the relative errors for the classical Levinson algorithm, Example 1.



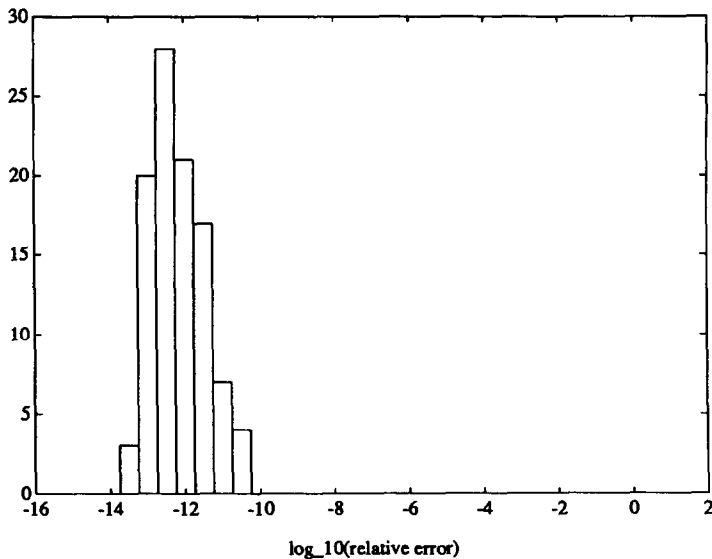


FIG. 3. Histogram of the relative errors for the look-ahead algorithm, Example 1.

matrices. We see that the relative errors are rather poor. In Figure 3, we plot the relative errors for the look-ahead Algorithm 6.1 (with  $h_{\max} = 2$ ). We see a substantial improvement of the relative errors. We remark that a run of the look-ahead Algorithm 6.1 with the recommended choice  $h_{\max} = 5$  gave the same results as for  $h_{\max} = 2$ .

**EXAMPLE 2.** This test set consists of 100 nonsymmetric  $200 \times 200$  matrices with at least one ill-conditioned leading principal submatrix. The matrices were generated as in Example 1. In Figure 4 and Figure 5, we plot the histograms of the relative errors for the classical Levinson algorithm and the look-ahead Algorithm 6.1 (with  $h_{\max} = 2$ ), respectively. In Table 2, we list, for both Example 1 and Example 2, the average number of multiplications required to solve one system in the test set by the classical Levinson algorithm and the look-ahead algorithm, and we state the corresponding overhead for the look-ahead algorithm.

**EXAMPLE 3.** This test set consists of symmetric matrices given by

$$t_0 = \varepsilon, \quad t_i = t_{-i} = \left(\frac{1}{2}\right)^i, \quad i = 1, 2, \dots, n. \quad (8.1)$$

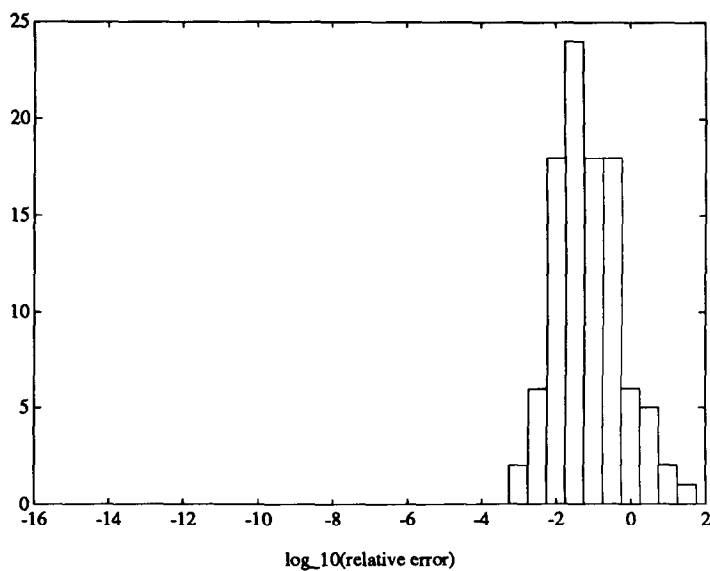


FIG. 4. Histogram of the relative errors for the classical Levinson algorithm, Example 2.

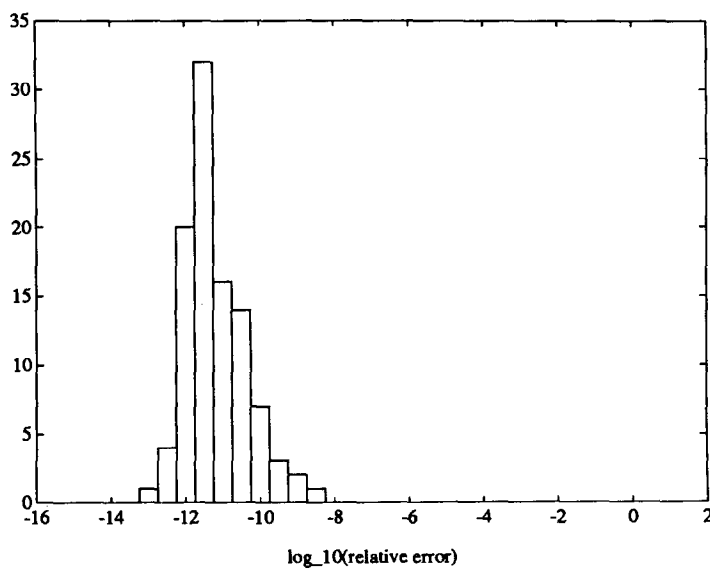


FIG. 5. Histogram of the relative errors for the look-ahead algorithm, Example 2.

TABLE 2  
AVERAGE NUMBER OF MULTIPLICATIONS FOR EXAMPLES 1 AND 2

$n + 1$	No. of multiplications		Overhead
	Classical	Look-ahead	
64	12,096	12,740	3.7%
200	119,400	120,010	3.5%

These are special cases of a class of Toeplitz matrices called Kac-Murdock-Szegő (KMS) matrices (with  $\rho = \frac{1}{2}$ ); see [29]. The eigenvalues of the KMS matrices (8.1) can be easily computed [45]. It turns out that, for  $\varepsilon = 0$ , each third principal submatrix, i.e.,  $T_{3m}$ ,  $m = 0, 1, \dots$ , is exactly singular, while the remaining submatrices are well conditioned. Consequently, if  $\varepsilon$  is set to a small number, then every third principal leading submatrix is ill-conditioned. The KMS matrices (8.1), with  $\varepsilon = 10^{-14}$ , were also used as test examples in [8], and we chose the same parameter  $\varepsilon = 10^{-14}$ . We ran the classical Levinson algorithm and the look-ahead Levinson Algorithm 7.1 (with  $h_{\max} = 2$ ) for KMS matrices  $T_n$  of order  $n + 1 = 15, 30, 60, 120, 240, 480$ . The relative errors and the numbers of multiplications are listed in Table 3. We see that the look-ahead procedures yields solutions with nearly full accuracy. Considering that one-third of the iteration steps are inner steps, the overhead of the look-ahead procedure is still reasonable.

EXAMPLE 4. This example is taken from [42], and it was also used in [9]. It is a  $13 \times 13$  matrix with five consecutive ill-conditioned leading principal

TABLE 3  
TEST RESULTS FOR THE KMS MATRICES, EXAMPLE 3

$n + 1$	Relative error		Multiplications		
	Classical	Look-ahead	Classical	Look-ahead	Overhead
15	0.0191	$1.20 \times 10^{-15}$	630	960	52%
30	0.0184	$1.79 \times 10^{-15}$	2,610	3,870	48%
60	0.0185	$1.98 \times 10^{-15}$	10,620	15,340	46%
120	0.0186	$4.61 \times 10^{-15}$	42,840	62,280	45%
240	0.0186	$6.85 \times 10^{-15}$	172,080	248,333	44%
480	0.0187	$3.69 \times 10^{-14}$	689,760	995,853	44%

TABLE 4  
ELEMENTS OF THE MATRIX IN EXAMPLE 4

t	5											
t1	-1	6	2	5.697	5.850	3	-5	-2	-7	1	10	-15
t2	1	-3	12.755	-19.656	28.361	-7	-1	2	1	-6	1	-0.5

submatrices. Its entries  $\{t_{j\bar{j}}\}_{\bar{j}=-13}^{13}$  are listed in Table 4, where

$$t := t_0, \quad t1 := \begin{bmatrix} t_{-1} & t_{-2} & \cdots & t_{-13} \end{bmatrix},$$

$$t2 := \begin{bmatrix} t_1 & t_2 & \cdots & t_{13} \end{bmatrix}.$$

The condition-number profile is shown in Table 5. We ran the standard Levinson algorithm and the look-ahead Algorithm 6.1 (with  $h_{\max} = 6$ ). The relative error of the classical algorithm was  $3.20 \times 10^{-10}$ ; the look-ahead algorithm generated the solution with relative error  $7.09 \times 10^{-14}$ .

EXAMPLE 5. Finally, we consider the symmetric  $7 \times 7$  matrix (7.6) from Section 7.2. The classical Levinson algorithm breaks down for this matrix, while the look-ahead Algorithm 7.1 (with  $h_{\max} = 4$ ) generates the exact

TABLE 5  
CONDITION-NUMBER PROFILE OF THE MATRIX IN EXAMPLE 4

$m$	$\kappa(T_m)$
0	2.00E - 1
1	1
2	1.63
3	9.45E + 5
4	2.40E + 6
5	3.61E + 5
6	4.76E + 6
7	3.60E + 6
8	3.34E + 2
9	1.71E + 2
10	1.63E + 1
11	4.02E + 1
12	2.05E + 1

TABLE 6  
CONDITION-NUMBER PROFILE OF THE MATRIX IN EXAMPLE 5

$m$	$\kappa(T_m)$
0	1.09E + 15
1	1.00
2	3.98E + 14
3	6.53E + 14
4	8.74E + 14
5	1.81E + 1
6	7.21

solution. Next, we perturbed the matrix slightly by adding a Toeplitz matrix with random entries in  $[-10^{-14}, 10^{-14}]$  to (7.6). The condition-number profile of the resulting matrix is shown in Table 6. Note that none of the submatrices are exactly singular. Nevertheless, the classical Levinson algorithm still breaks down. The look-ahead Algorithm 7.1 computes a solution with relative error  $1.33 \times 10^{-14}$ .

Finally, we remark that a slightly extended version of this paper is available as a technical report [15], and a few more numerical examples can be found there.

## 9. CONCLUDING REMARKS

We have studied formally biorthogonal polynomials (FBOPs) for bilinear forms induced by general Toeplitz matrices. We presented new recurrence relations that connect successive pairs in any given subsequence of all existing FBOPs. Based on these recursions, we proposed a look-ahead algorithm for solving general Toeplitz systems. This procedure is an extension of the classical Levinson algorithm for strongly regular Toeplitz matrices. We stress that our look-ahead algorithm is different from other generalizations of the Levinson algorithm that have been proposed. Except for the procedure devised by Chan and Hansen [9], all these algorithms can only skip over exactly singular submatrices. The algorithm in [9] allows one to skip over ill-conditioned submatrices; however, as we showed, the procedure can break down if two or more consecutive blocks of ill-conditioned submatrices occur. In contrast to these other proposed extensions of the Levinson algorithm, our look-ahead procedure skips over exactly singular, as well as ill-conditioned, leading principal submatrices, and it can handle arbitrary consecutive blocks of ill-conditioned submatrices. We reported results of numerical experiments,

which demonstrate that our look-ahead Levinson algorithm generates solutions of Toeplitz systems with ill-conditioned submatrices to nearly full accuracy.

We remark that similar techniques can be used to derive a look-ahead algorithm for solving general Hankel systems. A detailed description of such a look-ahead Hankel solver can be found in [16]. We stress that the Hankel case is fundamentally different from the Toeplitz case. The Hankel case is actually simpler in the sense that bilinear forms associated with Hankel matrices are always symmetric, and consequently one only has to deal with one sequence of *formally orthogonal polynomials* (FOPs), rather than two sequences of FBOPs as in the Toeplitz case. We note that FOPs associated with Hankel matrices are intimately connected with the nonsymmetric Lanczos process [35] for matrix computations; see, e.g., [14] and the references given there.

In future work, we intend to give a rigorous stability analysis of the look-ahead Levinson algorithm proposed in this paper. Furthermore, we plan to develop a software package with FORTRAN and MATLAB implementations of this algorithm, as well as the Hankel solver described in [16].

In recent years, various so-called superfast algorithms have been developed that solve Toeplitz systems with only  $O(n \log^2 n)$  operations; see, e.g., [1, 4, 5, 46]. Bunch [7] discussed the stability of some of these algorithms, and he pointed out that they are unstable in the case of general Toeplitz systems. It is natural to ask whether look-ahead techniques can also be used to enhance the stability of superfast Toeplitz solvers. This question is addressed in a recent paper by Gutknecht [22], who devised two superfast Toeplitz algorithms with look-ahead. However, no numerical results are given in [22], and it remains to be seen whether these algorithms can be turned into practical numerical procedures.

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